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(54) Title: CRYSTAL STRUCTURE OF BACE AND USES THEREOF

(57) Abstract: This invention is directed to the three dimensional crystal structure of Beta-site APP Cleaving Enzyme (BACE), and to the use of this structure in rational drug design methods to identify agents that may interact with active sites of BACE. Such agents may represent new therapeutics in the treatment and/or prevention of Alzheimer's Disease.

CRYSTAL STRUCTURE OF BACE AND USES THEREOF

Field of the Invention

[0001] The present invention relates to the three dimensional crystal structure of Beta-site APP Cleaving Enzyme (BACE), and to the use of this structure in rational drug design methods to identify agents that may interact with active sites of BACE. Such agents may represent new therapeutics in the treatment and/or prevention of Alzheimer's Disease.

Background of the Invention

[0002] A characteristic pathology of Alzheimer's Disease is the build up of insoluble amyloid plaques in the brain. These proteinaceous plaques are composed of a 4KDa, 42 amino acid fragment of β-Amyloid Precursor Protein (APP) and is termed Amyloid β -peptide (A β). The mechanism of A β production is hence of critical importance in understanding the onset and progress of Alzheimer's Disease. It has been shown that $A\beta$ is derived from the proteolytic cleavage of a larger protein, β -amyloid precursor protein (APP). Two enzymes are responsible for this cleavage; first, the enzyme β -secretase cleaves APP at residue 671 (770aa isoform of APP numbering) and then y-secretase cleaves at residue 716. More recently, the novel transmembrane aspartic protease BACE has been identified as being β -secretase. This protein is now a significant target in a therapeutic approach to Alzheimer's Disease. In rare cases of Alzheimer's Disease that are hereditary (Familial Alzheimer's Disease (FAD)) the disease phenotype has been isolated to mutations in the β -Amyloid Precursor Protein. One particular cohort, the 'Swedish mutation', exhibits a double mutation at the β -secretase cleavage site.

[0003] Based upon the role of BACE in Alzheimer's Disease, the elucidation of the three-dimensional structure of BACE, as well as its site of binding with APP, would have important implications in the treatment and/or prevention of Alzheimer's Disease and similar diseases associated with the

presence of insoluble amyloid plaques composed the 42 amino acid fragment of APP in the brain.

Summary of the Invention

The present invention provides a crystal of BACE complexed with an APP inhibitor peptide, as well as the three dimensional structure of BACE as derived by x-ray diffraction data of the BACE/APP inhibitor peptide crystal. Specifically, the three dimensional structure of BACE is defined by the structural coordinates shown in Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. The structural coordinates of BACE are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of various active sites of BACE, and the BACE/APP inhibitor peptide complex, including the APP binding site. The active site structures may then be used to design various agents which interact with BACE, as well as BACE complexed with an APP protein or peptide, or related molecules.

[0005] The present invention is also directed to an active site of an APP binding protein or peptide, and preferably the APP peptide binding site of BACE that is elucidated and derived from the three dimensional structure of BACE as defined by the relative structural coordinates set forth in Figure 1, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

In one embodiment of the present invention, the active site of the APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

[0007] In another embodiment, the active site of the APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the

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relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

[0008] The present invention further provides a method for identifying an agent that interacts with an active site of BACE. The method comprises the steps of: (a) determining a putative active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, \pm a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å; and (b) performing various computer fitting analyses to identify an agent which interacts with the putative active site.

[0009] The present invention also provides method for identifying an agent that interacts with an active site of an APP binding protein or peptide, preferably BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and (b) designing an agent using the three dimensional model generated in step (a).

The present invention also provides another method for [0010] identifying an agent that interacts with an active site of an APP binding protein or peptide, preferably BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and (b) designing an agent using the three dimensional model generated in step (a):

[0011] Finally, the present invention provides agents, and preferably inhibitors, identified using the foregoing methods. Small molecules or other agents which inhibit or otherwise interfere with the ability of BACE to cleave APP may be useful in the treatment and/or prevention of Alzheimer's Disease.

[**0012**] Additional objects of the present invention will be apparent from the description which follows.

Brief Description of the Figure

[0013] Figure 1 provides the atomic structural coordinates for BACE and the APP inhibitor peptide as derived by X-ray diffraction of a crystal of the BACE and APP inhibitor peptide complex. "Atom type" refers to the atom whose coordinates are being measured. "Residue" refers to the type of residue of which each measured atom is a part - i.e., amino acid, cofactor, ligand or solvent. The

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"x, y and z" coordinates indicate the Cartesian coordinates of each measured atom's location in the unit cell (\mathring{A}). "Occ" indicates the occupancy factor. "B" indicates the "B-value", which is a measure of how mobile the atom is in the atomic structure (\mathring{A}^2).

Detailed Description of the Invention

[0014] As used herein, the following terms and phrases shall have the meanings set forth below:

Inless otherwise noted, "BACE" is Beta-site APP Cleaving Enzyme, and is the β-secretase enzyme that cleaves β-amyloid precursor protein (APP) at residue 671 (770aa isoform of APP numbering). After cleavage of APP by BACE, the remaining APP is cleaved at residue 716 by γ-secretase, leaving a 42 amino acid fragment of APP that is found in the proteinaceous plaques of Alzheimer's patients. The amino acid sequence of BACE preferably has the amino acid sequence deposited with Swiss Prot under accession number P56817, including conservative substitutions. As used herein, BACE also includes "BACE peptides," which are molecules having less than the complete amino acid sequence of BACE. Preferably, BACE peptides include the active site in which BACE binds to and cleaves APP. Most preferably, the BACE peptide corresponds to amino acid residues 58-447 set forth in Figure 1 ("BACE₅₈₋₄₄₇"), including conservative substitutions.

[0016] "APP" is β -amyloid precursor protein having the amino acid sequence deposited with Swiss Prot under accession number CAA31830, including conservative substitutions. As used herein, APP also includes "APP peptides," which are molecules having less than the complete amino acid sequence of APP. Preferably, APP peptides include the active site in which APP is cleaved by BACE.

[0017] An "APP inhibitor peptide" is a peptide which inhibits binding between BACE and APP. Preferably, the APP peptide has the amino acid sequence SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE, where Sta is rare amino acid (S)-Statine.

[**0018**] An "APP binding protein or peptide" is a protein or peptide that binds APP and has a APP binding site, and includes but is not limited to BACE and BACE peptides.

[0019] Unless otherwise indicated, "protein" shall include a protein, protein domain, polypeptide or peptide.

[0020] "Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using x-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original set provided in Figure 1 by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Figure 1.

[**0021**] An "agent" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound or drug.

"Root mean square deviation" is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates of BACE described herein. The present invention includes all embodiments comprising conservative substitutions of the noted amino acid residues resulting in same structural coordinates within the stated root mean square deviation.

[0023] The numbering of the amino acid residues identified in Figure 1 are based on the numbering of the full length BACE protein from the start of the signal sequence. It will be obvious to the skilled practitioner that the numbering of the amino acid residues of BACE may be different than that set forth herein or may contain certain conservative amino acid substitutions that yield the same

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three dimensional structures as those defined in Figure 1. Corresponding amino acids and conservative substitutions in other isoforms or analogues are easily identified by visual inspection of the relevant amino acid sequences or by using commercially available homology software programs (e.g., MODELLAR, MSI, San Diego, CA).

[0024] "Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic) and includes substitutions having an inconsequential effect on the three dimensional structure of BACE, with respect to the use of this structure for the identification and design of agents which interact with BACE, for molecular replacement analyses and/or for homology modeling.

[0025] As used herein, an "active site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug) via various covalent and/or non-covalent binding forces. Preferably, the active site of BACE corresponds to the site in which BACE cleaves the APP molecule.

[0026] As such, the active site of BACE may include, for example, both the actual site in which BACE binds and cleaves APP, as well as accessory binding sites adjacent or proximal to the actual binding site that nonetheless may affect the ability of BACE to bind and cleave APP, either by direct interference with the actual site of binding or by indirectly affecting the steric conformation or charge potential of the BACE molecule and thereby preventing or reducing the ability of BACE to bind to APP at the actual binding site. As used herein, an active site also includes BACE or BACE analog residues which exhibit observable NMR perturbations in the presence of a binding ligand, such as APP or an APP peptide. While such residues exhibiting observable NMR perturbations may not necessarily be in direct contact with or immediately

proximate to ligand binding residues, they may be critical to BACE residues for rational drug design protocols.

[**0027**] The present invention is directed to a crystallized complex of BACE and an APP inhibitor peptide that effectively diffracts X-rays for the determination of the structural coordinates of the complex. As used herein, BACE preferably corresponds to BACE₅₈₋₄₄₇ as set forth in Figure 1, with the N-terminal domain consisting of amino acid residues 58-207 shown in Figure 1, and the C-terminal domain consisting of amino acid residues 208-447 shown in Figure 1. The APP inhibitor peptide is preferably SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE.

[0028] Using the crystal complex of the present invention, X-ray diffraction data can be collected by a variety of means in order to obtain the atomic coordinates of the crystallized molecule or molecular complex. With the aid of specifically designed computer software, such crystallographic data can be used to generate a three dimensional structure of the molecule or molecular complex. Various methods used to generate and refine the three dimensional structure of a crystallized molecule or molecular structure are well known to those skilled in the art, and include, without limitation, multiwavelength anomalous dispersion (MAD), multiple isomorphous replacement, reciprocal space solvent flattening, molecular replacement, and single isomorphous replacement with anomalous scattering (SIRAS).

[0029] Accordingly, the present invention also provides the three dimensional structure of BACE as derived by x-ray diffraction data of the BACE/APP inhibitor peptide crystal. Specifically, the three dimensional structure of BACE is defined by the structural coordinates shown in Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å, preferably not more than 1.0Å, and most preferably not more than 0.5Å. The structural coordinates of BACE are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of various active sites of BACE, and the BACE/APP inhibitor peptide complex, including the APP or APP peptide binding site. The active site

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structures may then be used to design agents with interact with BACE, as well as BACE complexed with APP, an APP peptide or related molecules.

[0030] The present invention is also directed to an active site of an APP binding protein or peptide, preferably the APP peptide binding site of BACE, which comprises the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

[0031]In another preferred embodiment, the active site of an APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

[0032] Another aspect of the present invention is directed to a method for identifying an agent that interacts with an active site of BACE comprising the steps of: (a) determining an active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than

1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å; and (b) performing computer fitting analysis to identify an agent which interacts with said active site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the putative active site and the identified agent, by (a) generating a three dimensional model of the putative active site of a molecule or molecular complex using homology modeling or the atomic structural coordinates of the active site, and (b) determining the degree of association between the putative active site and the identified agent. Three dimensional models of the putative active site may be generated using any one of a number of methods known in the art, and include, but are not limited to, homology modeling as well as computer analysis of raw data generated using crystallographic or spectroscopy data. Computer programs used to generate such three dimensional models and/or perform the necessary fitting analyses include, but are not limited to: GRID (Oxford University, Oxford, UK), MCSS (Molecular Simulations, San Diego, CA), AUTODOCK (Scripps Research Institute, La Jolla, CA), DOCK (University of California, San Francisco, CA), Flo99 (Thistlesoft, Morris Township, NJ), Ludi (Molecular Simulations, San Diego, CA), QUANTA (Molecular Simulations, San Diego, CA), Insight (Molecular Simulations, San Diego, CA), SYBYL (TRIPOS, Inc., St. Louis. MO) and LEAPFROG (TRIPOS, Inc., St. Louis, MO).

I 0033] The present invention also provides a method for identifying an agent that interacts with an active site of an APP binding protein or peptide, and preferably the APP peptide binding site on BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å;

and (b) designing an agent using the three dimensional model generated in step (a). In another preferred embodiment, the active site of the APP binding protein or peptide is generated using the three dimensional model defined by the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96. SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

The effect of such an agent identified by computer fitting analyses [0034]on the APP binding protein or peptide may be further evaluated by obtaining or synthesizing the agent, and contacting the identified agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide. Preferably, the APP binding protein or peptide is BACE (or a BACE peptide), and the agent is a potential inhibitor of binding between BACE (or a BACE peptide) and APP (or an APP peptide). Therefore, in the preferred embodiment, the agent is contacted with BACE (or a BACE peptide) in the presence of APP (or a APP peptide), to determine the ability of the agent to inhibit binding between BACE (or the BACE peptide) and APP (or the APP peptide). Depending upon the action of the agent on the active site, the agent may act either as an inhibitor or activator of the BACE/APP binding. Assays may be performed and the results analyzed to determine whether the agent is an inhibitor (i.e., the agent may reduce or prevent binding affinity between BACE and APP), an activator (i.e., the agent may increase binding

affinity between BACE and APP), or has no effect on the interaction between BACE and APP. Agents identified using the foregoing methods, and preferably inhibitors of BACE cleavage of APP, may then be tested as therapeutics in the treatment and/or prevention of Alzheimer's Disease, and other diseases that are also characterized by the presence of the 42 amino acid fragment of APP in the proteinaceous plaques of the brain.

[0035] Various molecular analysis and rational drug design techniques are further disclosed in U.S. Patent Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published WO 99/09148, the contents of which are hereby incorporated by reference.

[0036] Finally, the present invention is also directed to the agents, and preferably the inhibitors, identified using the foregoing methods. Such agents may be a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, or drug, and preferably are small molecules that effectively inhibit binding between BACE and APP or an APP peptide. Such molecules may be useful in treating, preventing or inhibiting progression of Alzheimer's Disease.

[0037] The present invention may be better understood by reference to the following non-limiting Example. The following Example is presented in order to more fully illustrate the preferred embodiments of the invention, and should in no way be construed as limiting the scope of the present invention.

Example 1 with the second seco

A Methods

[0038] Cloning of Human BACE1. Human polyA+ mRNA from whole brain (Clontech) was converted to cDNA by random-priming using Thermoscript RT-PCR System, according to the manufacturer's protocol (Lifetechnologies). This cDNA was amplified by PCR using the forward and reverse primers, 5' GCTCTAGAACCCAGC ACGGCATCCGGCTG 3' (XbaI site indicated by underlined sequence; nts. 517-537 in accession no. AF190725) and 5' CCAAGCATGCGGCCGCAATAGGCTATGGTCA TGAGGGTTGAC 3' (NotI site

indicated by underlined sequence; nts. 1809-1833; bold "A" indicates additional nucleotide to permit in-frame translation of the Fc chimera; see below), respectively. PCR was accomplished using Expand Long Polymerase kit according to the manufacturer's conditions (Roche Biochemicals; buffer #3), with PCR cycling consisting of an initial denaturing step at 95°C for 3min, 30-40 cycles of denaturation at 94°C for 30sec, annealing at 65°C for 30sec, elongation at 68°C for 1min 30sec, followed by a final elongation at 68°C for 5min. The PCR products were run on a 1% agarose gel. The appropriate band was cut out of the gel, purified by Quantum Prep Freeze 'N Squeeze DNA Extraction Columns (Bio-Rad), and cloned into the Spel/NotI sites of the mammalian expression vector, pED/Fc (Kaufman, RJ et al., 1991, Nucl. Acids. Res. 19:4485-4490).

[0039]An intermediate construct contained the honey bee meletin secretory leader fused to the the prodomain and coding region of BACE1, just upstream to the predicted transmembrane domain of BACE1 (Vassar, R. et al., 1999, Science 286:735-741). The absence of the predicted hydrophobic transmembrane domain in this construct would permit soluble secreted BACE.Fc protein to be extracted from the conditioned medium. Downstream of BACE1 was an engineered enterokinase cleavage site followed by sequence encoding the Fc portion of immunoglobulin IgG. The final construct contained the BACE1.Fc gene, flanked by SalI and EcoRI in pED/Fc, cloned into the SalI/EcoRI sites of the mammalian expression vector, pHTop, a derivative of pED, in which the majority of the adenovirus major late promoter was replaced by six repeats of a bacterial tetracycline operator (described in Gossen et al, 1992, PNAS, 89:5547-5551). Sequencing of the BACE1.Fc recombinant gene was accomplished by BigDye terminator dideoxy sequencing using an ABI3700. Sequence analyses was accomplished using DNAstar software package.

[0040] Expression of Human BACE1. The vector, pHTOP, with the BACE1.Fc insert, contains the dihydrofolate reductase gene and when introduced in the cell line CHO/A2 (see description below) functions very

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efficiently and high expressers can be selected by isolating cells surviving in high methotrexate concentrations. The CHO/A2 cell line is derived from CHO DUKX B11 (Urlaub and Chasin, 1980, PNAS USA 77:4216-4220) by stably integrating a transcriptional activator (tTA), a fusion protein between the Tet repressor and the herpes virus VP16 transcriptional domain (Gossen et al). A CHO cell line expressing extracellular BACE1. Fc was established by transfecting (lipofection) pHTopBACE1. Fc into CHO/A2 cells and selecting clones in 0.02 and 0.05 μ M methotrexate. The conditioned media from multiple clones were screened by Western blot using a (mouse) anti-human IgG. Fc HRP antibody. The same clones were also metabolically labeled with 35 S (met/cys). The best clone, determined by virtue of its high expression, was one which resulted from 0.05 μ M MTX selection and was chosen to be scaled up for roller bottle conditioned media production (4 Liters). The conditioned media was then used for purification. The expressed protein has residues 22-460 and nine extra residues at the C-terminal (an artefact from cloning and remains of the EK cleavage site).

[0041] Purification of BACE1. For the purification of BACE the 102 liters of conditioned media was used. During purification the activity of the enzyme was estimated at room temperature by continuously monitoring the fluorescent intensity for 5-10 min. at 420 nm (ext – 320 nm) Abz-Ser-Glu-Val-Asn-Leu-Asp-Ala-Glu-Phe-Arg-Dpa (Abz = Amino benzoic acid, Dpa = 9,10-diphenylanthracene) as the substrate. The reaction mixture contained 20 μ M of substrate, different amounts of enzyme in 0.5 ml of 20 mM Tris-HCl pH 8.0 and 100 mM NaCl. The concentrated material of conditioned media(1.6 l) was applied to column (2.8 x 12 cm) containing ImmunoPure Immobilized Protein A agarose (Pierce, Il, USA) equilibrated in PBS buffer. The speed of application was 2 ml/min. The column was washed with 1 litre of PBS buffer and the BACE-Fc protein was eluted by ImmunoPure IgG Elution Buffer (Pierce, Il, USA). The fractions containing protein were immediately neutralized by 1 M Tris-HCl to pH 8.0.

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[0042] The obtained protein material was treated with Enterokinase at 25°C. The ratio of BACE-Fc to Enterokinase was 3000:1 and the time of reaction was 3 hrs. The reaction was stopped by removing Enterokinase from reaction mixture by applying the protein to a column (1 x 5 cm) containing soybean trypsin inhibitor agarose (Sigma, Mo, USA) equilibrated in 20 mM Tris-HCL pH 8.0 containing 100 mM NaCl (speed was 1 ml/min). The flow through material contained BACE and cleaved Fc. Cleaved Fc was removed from BACE by flowing through a protein A column equilibrated in 20 mM Tris-HCl pH 8.0. [0043] BACE was partially de-glycosylated using PNGase F (New England Labs., Ma, USA). 8-9 µg of PNGase was added to 1 mg of BACE and the incubation was carried at 37° C for 16 hrs. The additional 5-6 µg of PNGase was added to each mg of BACE and incubation was continued for another 4 hrs. The purified BACE was separated from PNGase by HPLC size-exclusion chromatography using 21.5 x 30 cm G-3000SW column (TosoHaas, Pa, USA) equilibrated in 20 mM tris-HCL pH 8.0 containing 200 mM NaCl. (Speed of elution was 3 ml/min). The purified BACE was concentrated and used for crystallization experiments.

[0044] N-terminal sequencing of purified BACE reveals a mixture of protein species, with the major sample having the processing domain cleaved and beginning at residue 47 (all numbering refers to full length BACE; accession code: A59090) and a minor sample which had not been cleaved beginning at residue 22. A smaller sample with sequence MTIAY was also detected.

Crystallization. The crystals were grown using the hanging drop vapour diffusion method. The protein was concentrated to mg/ml in 20mM Tris pH 7.5, 200mM sodium chloride. Inhibitor peptide sequence is SEVNStaVAEF, where Sta is the rare amino acid (S)-Statine. It was concentrated to 100mM in 100% DMSO and mixed with concentrated protein in a two-fold peptide excess to form the complex. 1 μ l of complex was added to 1 μ l of well solution containing 100mM Sodium Cacodylate pH6.5, 25% PEG8K, 300mM lithium sulphate. Plate-like crystal clusters grew within one week to dimensions of 200

 μ m x 400 μ m x 75 μ m. Single crystals were transferred to a stabilizing, cryoprotectant solution which contained the well solution plus 25% Glycerol for a brief, 10 second, soak and then frozen in liquid nitrogen. X-ray diffraction crystals had space group I222, and unit cell parameters a=86.627, b=130.861, c=130.729, and α = β = γ =90°.

B. Results

E 0046] Structure Determination and Overall Fold. Full length BACE was expressed in CHO cells as a fc fusion protein and, after purification, cleavage and partial deglycosylation, complexed with peptide inhibitor and crystallized. Crystals diffracted to 2.3Å and the structure was solved using the technique of molecular replacement. The search model used was derived from cod atlantic Pepsin and contained 63% of the final number of atoms. The density modified maps obtained using a poly-alanine version of the search model (39% of the final atoms) provided sufficient information to build all but 12 amino acids. The final model contains residues from 59 to 448 (using full length numbering), all 9 residues of the statine inhibitor and 360 water molecules. Of the four predicted N-linked glycosylation sites only two have interpretable electron density.

[0047] The overall shape of the BACE protein is spherical and is composed of two distinct domains, an N-terminal (58-207) and a C-terminal (208-447). With the first thirteen amino acids (58-71) being packed against residues 238-243. There is a significant cleft-like channel across one surface of the interface between the domains. This contains the inhibitor peptide and conserved aspartic acid motifs that define the active sites of aspartic proteases.

[0048] The N-terminal domain is composed of a single a-helix preceeding the loop joining the two domains and thirteen β -strands. The larger C-terminal domain has a total of seventeen β -strands and three α -helices. The overall topology is characterised by an eight stranded antiparallel interdomain β -sheet. This central sheet comprises the majority of the active site residues including the two conserved aspartates (one from each domain:93 and 289). Asp93 and

Asp289 define the position of a pseudo two-fold axis for the central β -sheet. Outside of this symmetry the two domains differ significantly. The N-terminal domain has an extra two strands extending the central sheet. In addition, there are two anti-parallel β -sheets above and below the central sheet composed of three and four β -strands respectively. Residues from the upper sheet (131-135) fold over the active site aspartates and form a 'flap' over the centre of the peptide binding cleft.

[0049] The C-terminal domain contains two lobes in addition to the strands which from the central β -sheet. These are weakly homologous to known aspartic protease structures. The binding pocket for the P1` and P3` positions are instead derived from three β -turns 388-391, 284-286 and 255-261.

[0050] There are a total of six cysteine residues in BACE. Each of these is involved in a disulphide interaction. The pattern of disulphide crosslinking, Cys278-Cys443, Cys380-Cys330, Cys420-Cys216 are unique in the aspartic proteases known to date.

[0051] A novel aspartic protease. The first attempts to study the relationship of function to structure of an Apartic proteases began in the 1930s with Pepsin. Since then this rich field of research has been successfully applied to the design of clinically used inhibitors in only one system; HIV protease. The reasons for this are related more to the validity of the pharmacological target than the efficacy of inhibitors. β -secretase has been described as a novel protease and has been shown to be linked to the onset and progression of Alzheimer's disease.

[0052] From a gross viewpoint the overall fold and domain organization is very similar to that of a canonical aspartic protease. The comparison at a more detailed level reveals a significant number of differences. The active site is characterized by two aspartic residues surrounded by a conserved set of hydrogen bonds termed a 'fireman's grip'. This is reproduced in the -secretase structure presented here. The characteristic flap which wraps over the active site in pepsin is absent from the C-terminal domain in a manner analogous to

cathepsin D. In β -secretase the critical main chain amide hydrogen bond to the carboxyl group of statine is maintained by Thr133 from this flap. The amide of the statine makes a hydrogen bond to the carboxyl group of Gly95, emphasizing that the statine residue occupies both the P1 and P1` position.

Enzyme Mechanism. It has been shown that $\beta\mbox{-secretase}$ cleavage [0053]is dependent on proximity to the cell membrane. Both β -secretase and its substrate APP have putative transmembrane regions. Our expressed BACE construct finishes one amino acid before the predicted transmembrane region. The final residue in the current structure is Ile447, thirteen residues away from the beginning of the putative transmembrane domain. In the current crystal structure Ile447 is only 6Å away from the P3 Glutamic acid of the inhibitor suggesting a role for the remaining C-terminal residues in the enzyme mechanism. The Statine residue of the inhibitor peptide is bound at the S1 position within the active site. The position of the C-3 hydroxyl group, coplanar to and within hydrogen bonding distance of both aspartate 93 and 289 carboxyl groups, confirms that the rare amino acid mimics the tetrahedral transition state i.e the intermediate of peptide-bond hydrolysis. The distance between the oxygen atoms of Asp93 and Asp289 is 2.8Å, strongly suggesting a shared proton atom and a classic aspartic protease pK profile for these side-chains and a common enzyme mechanism to other known aspartic proteases.

Inhibitor binding. The inhibitor peptide binds in an extended form along a 20Å groove formed at the interface between the domains. The conserved catalytic aspartic residues lie at the middle of this groove. The bound peptide consists of 8 amino acids plus a statine amino acid at position 5. There is contiguous electron density for the whole peptide. The statine based inhibitor used in this study has been show to inhibit the β -secretase enzyme with nanomolar efficiency. The peptide sequence is based on the P10 to P4` APP751 Sweedish family mutation. This mutation of a Lys-Asn at the P2 position and Met-Leu at the P1 position is strongly correlated to the early onset of

Alzheimer's disease. The inhibitor peptide utilizes Statine's Leucyl like side-chain to explore this interaction. Due to the di-peptide nature of Satine the P1' position of the substrate is shifted to P2' leaving an empty S1' pocket. The β -secretase enzyme appears to have a novel preference for an apartate or glutamate at the P1' position whereas other aspartic proteases show a preference for hydrophobic residues. This unusual preference for a negatively charged P1' amino acid is explained by the guanadinium group of Arg189 forming part of the putative S1' pocket. Even at the acidic pH optima of BACE the arginine side chain would form a positively charged environment for the possibly protonated carboxyl side-chain atoms.

[0055] The S1 and S3 binding pockets are a contiguous, hydrophobic pocket formed by the side-chain of residues Tyr132, Phe169, Ile171, Trp176, Ile179 and main chain atoms of Gly74, and Gln73. This packing of inhibitor P1 and P3 side chains has been seen in previous aspartic protease complexes.

[0056] The canonical APP cleavage site for b-secretase appears to have a preference for a small hydrophobic residues at the P2` position. The side chain of the valine residue bound in the putative S2` site of β -secretase appears to not make any significant interactions with the protein, its main chain however forms a tight set of hydrogen bonds to the backbone carboxyl of Gly 95 and the sidechain OH of Tyr259. In turn, Tyr259 is held rigidly in place by an edge-pi interaction with Trp258, which packs against the guanadinium group of Arg256.

[0057] Swedish mutation. Autosomal dominant mutations identified on the β -amyloid precusor protein have been correlated to early-onset cases of Alzheimer's disease. These have been shown to cluster around the three canonical cleavage sites. A double (the so-called Swedish) mutation of Lys670-Met671 (770aa isoform of APP numbering) to Asn-Leu causes an increase in the overall quantity of $A\beta$ detectable in the plasma and in the medium of cultured fibroblasts from carriers of the Swedish mutation. These two amino acids lie at the P2 and P1 positions of the β -secretase active site. The statine based inhibitor used here is based on this Swedish mutation. A methionine at position

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P1 would clearly be accommodated but would loose the van Der Waal's complentarity exhibited by the statine side-chain to Leu90 and Ile178. The C∈ atom of the methione would make supplement the hydrophobic interaction to Phe169.

Table 1

Residues of BACE Within 4Å of Peptide Inhibitor SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296, ARG368

Residues of BACE Within 8Å of Peptide Inhibitor
LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94,
GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133,
GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171,
ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183,
TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191,
ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286,
ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294,
LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383,
ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391,
THR392, VAL393, GLY395, ALA396, ILE447

[0058] All publications mentioned herein above, whether to issued patents, pending applications, published articles, deposited sequences, or otherwise, are hereby incorporated by reference in their entirety. While the foregoing invention has been described in some detail for purposes of clarity and understanding, it will be appreciated by one skilled in the art from a reading of the disclosure that various changes in form and detail can be made without departing from the true scope of the invention in the appended claims.

What is claimed is:

- 1. A crystallized complex of Beta-site APP Cleaving Enzyme (BACE) and SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE.
- 2. The crystallized complex of Claim 1, wherein BACE has an N-terminal domain consisting of amino acid residues 58-207 shown in Figure 1, and a C-terminal domain consisting of amino acid residues 208-447 shown in Figure 1.
- 3. An active site of an APP binding protein or peptide comprising the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 4. The active site of Claim 3, wherein the ± a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 5. The active site of Claim 3, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 6. An active site of an APP binding protein or peptide comprising the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171,

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ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

- 7. The active site of Claim 6, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 8. The active site of Claim 6, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 9. A method for identifying an agent that interacts with an active site of Beta-site APP Cleaving Enzyme (BACE), comprising the steps of:
- (a) determining an active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) performing computer fitting analysis to identify an agent which interacts with said active site.
- 10. The method of Claim 9, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 11. The method of Claim 9, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.

- 12. A method for identifying an agent that interacts with an active site of an APP binding protein or peptide, comprising the steps of:
- (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) designing an agent using the three dimensional model generated in step (a).
- 13. The method of Claim 12, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 14. The method of Claim 12, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 15. The method of Claim 12, wherein the agent is designed by performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- 16. The method of Claim 12, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.

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- 17. The method of Claim 12, wherein the APP binding protein or peptide is BACE.
- 18. The method of Claim 17, wherein the agent is a potential inhibitor of binding between BACE and APP.
- 19. The method of Claim 18, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with BACE in the presence of APP.
- 20. A method for identifying an agent that interacts with an active site of an APP binding protein or peptide, comprising the steps of:
- (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) designing an agent using the three dimensional model generated in step (a).
- 21. The method of Claim 18, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.

- 22. The method of Claim 20, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 23. The method of Claim 20, wherein the agent is designed by performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- 24. The method of Claim 20, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.
- 25. The method of Claim 20, wherein the APP binding protein or peptide is BACE.
- 26. The method of Claim 25, wherein the agent is a potential inhibitor of binding between BACE and APP.

27. The method of Claim 26, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with BACE in the presence of APP.

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- 28. An agent identified by the method of Claim 9.
- 29. An agent identified by the method of Claim 12.
 - 30. An agent identified by the method of Claim 20.

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Figure 1

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MOTA	1	Type	≘ GLY	Δ	58		31.563	49.775	16.324	1 00	59.33
ATOM	2	CA	GLY		58		32.861	50.358	16.764		58.44
ATOM	3	C	GLY		58		33.594	49.446	17.727		57.81
ATOM	4	0	GLY		58		34.067	48.331	17.333		56.66
	5				59		33.712	49.888	18.975	1.00	56.66
ATOM		N C2	SER				34.391	49.094	20.015		55.45
ATOM	6	CA	SER		59						53.77
ATOM	7	C	SER		59		33.560	49.088	21.293		54.40
ATOM	8	0	SER		59		32.978	50.147	21.704		
ATOM	9	CB	SER		59 50		35.781	49.668	20.309		55.79
ATOM	10	OG	SER		59			50.952	20.899	1.00	
ATOM	11	N	PHE		60		33.480	47.924	21.927	1.00	
MOTA	12	CA	PHE		60		32.719	47.772	23.181		45.72
ATOM	13	C	PHE		60		33.681	47.269 46.160	24.247		44.79 45.45
MOTA	14	0	PHE		60		33.495		24.831	1.00	43.45
ATOM	15	CB	PHE		60		31.564	46.790	22.976		43.28
ATOM	16	CG	PHE		60		30.557	47.249	21.957		40.54
ATOM	17		PHE		60		30.875 29.301	47.267	20.602		40.58
ATOM	18	CD2		A	60 60		29.301	47.701 47.731	22.355 19.658		39.88
ATOM	19	CE2	PHE		60		28.375	48.166	21.419		39.50
ATOM	20	CZ	PHE		60		28.704	48.182	20.070	1.00	39.23
ATOM	21 22		VAL		61		34.709	48.073	24.500	1.00	
ATOM		N	VAL		61		35.763	47.756	25.483		43.19
ATOM	23	CA C	VAL		61		35.763	47.069	26.738		41.81
ATOM ATOM	24 25	0	VAL		61		35.876	46.099	27.247		42.54
ATOM	25 26	CB	VAL		61		36.532	49.035	25.895	1.00	
	27		VAL		61		37.069	49.730	24.655	1.00	
MOTA	28		VAL		61		35.621	49.975	26.676		44.28
ATOM ATOM	29	N	GLU		62		34.114	47.542	27.252		40.86
ATOM	30	CA	GLU		62		33.517	46.959	28.470	1.00	
ATOM	31	C	GLU		62		33.208	45.473	28.320		36.45
ATOM	32	Ö	GLU		62		33.366	44.685	29.301		36.49
ATOM	33	CB	GLU		62		32.226	47.700	28.832		43.76
ATOM	34	CG	GLU		62		32.399	48.895	29.764	1.00	
ATOM	35	CD	GLU		62		32.743	48.486	31.188	1.00	
ATOM	36	OE1			62		32.317	47.387	31.612	1.00	53.41
ATOM	37		GLU		62		33.423	49.271	31.890	1.00	53.64
ATOM	38	N	MET		63		32.780	45.062	27.129	1.00	30.86
ATOM	39	CA		A	63		32.421	43.643	26.896		27.79
ATOM	40	C		A	63		33.491	42.741	26.279	1.00	26.02
ATOM	41	ō	MET	A	63		33.354	41.476	26.310	1.00	25.25
ATOM	42	CB	MET		63		31.130		26.078		25.63
ATOM	43	CG	MET		63		29.942	44.133	26.858	1.00	24.89
ATOM	44	SD	MET		63		28.392	44.180	25.960	1.00	23.85
ATOM	45	CE	MET	A	63		28.431	45.848	25.316	1.00	24.18
ATOM	46	N	VAL	Α	64		34.551	43.330	25.736	1.00	23.39
ATOM	47	CA	VAL	Α	64		35.639	42.516	25.143	1.00	20.76
ATOM	48	С	VAL		64		36.263	41.634	26.216	1.00	20.06
ATOM	49	0	VAL		64		36.531	42.095	27.370	1.00	18.87
ATOM	50	СВ	VAL		64		36.740	43.407	24.517		21.16
ATOM	51		VAL		64		37.958	42.567	24.151		18.99
ATOM	52		VAL		64		36.193	44.092	23.266	1.00	21.01
ATOM	53	N	ASP		65		36.487	40.373	25.869		18.21
ATOM	54	CA	ASP		65		37.091	39.397	26.800		18.56
ATOM	55	С	ASP		65		36.280	39.174	28.071		17.80
ATOM	56	Ō	ASP		65		36.869	38.964	29.165	1.00	16.29
ATOM	57	CB	ASP		65		38.508	39.829	27.194	1.00	21.53
MOTA	58	CG	ASP		65	,	39.409	40.055	25.993	1.00	22.65

a mon	59	OD1	ASP A	65		39.162	39.451	24.930	1.00 23.75
MOTA							40.831	26.117	1.00 24.72
MOTA	60		ASP A	65		40.375			
ATOM	61	N	ASN A	66		34.955	39.209	27.969	1.00 16.59
MOTA	62	CA	ASN A	66		34.090	38.987	29.156	1.00 16.58
ATOM	63		ASN A	66		33.719	37.508	29.274	1.00 17.20
						32.815	37.125	30.070	1.00 19.23
MOTA	64		ASN A	66					
MOTA	65	CB	ASN A	66		32.817	39.845	29.059	1.00 14.62
MOTA	66	CG	ASN A	66		31.967	39.516	27.835	1.00 15.57
MOTA	6.7	OD1	ASN A	66		32.381	38.714	26.937	1.00 16.31
	68		ASN A	66		30.788	40.120	27.760	1.00 14.85
ATOM							36.664	28.515	1.00 17.73
MOTA	69	N	LEU A	67		34.409			
MOTA	70	CA	LEU A	67		34.134	35.206	28.529	1.00 17.36
MOTA	71	С	LEU A	67		35.295	34.328	28.985	1.00 16.04
MOTA	72	0	LEU A	67		36.499	34.701	28.842	1.00 16.38
ATOM	73	СВ	LEU A	67		33.707	34.757	27.128	1.00 17.19
						32.226	34.504	26.839	1.00 18.63
MOTA	74	CG	LEU A	67					
ATOM	75	CD1	LEU A	67		31.349	35.604	27.407	1.00 16.94
MOTA	76	CD2	LEU A	67		32.049	34.375	25.330	1.00 18.67
MOTA	77	N	ARG A	68		34.956	33.166	29.531	1.00 14.58
ATOM	78	CA	ARG A	68		35.961	32.173	29.973	1.00 16.73
		C	ARG A	68		35.394	30.775	29.717	1.00 15.78
MOTA	79							29.500	1.00 13.85
MOTA	80	0	ARG A	68		34.154	30.610		
MOTA	81	CB	ARG A	68		36.299	32.349	31.459	1.00 18.19
ATOM	82	CG	ARG A	68		37.086	33.623	31.766	1.00 21.67
MOTA	83	CD	ARG A	68		37.571	33.646	33.213	1.00 23.25
MOTA	84	NE	ARG A	68		36.462	33.653	34.165	1.00 26.34
							33.500	35.482	1.00 27.29
MOTA	85	CZ	ARG A	68		36.598		•	
MOTA	86	NH1	ARG A	68		37.802	33.324	36.015	
MOTA	87	NH2	ARG A	68		35.530	33.527	36.271	1.00 26.77
ATOM	88	N	GLY A	69		36.262	29.769	29.726	1.00 14.89
ATOM	89	CA	GLY A	69		35.816	28.409	29.486	1.00 15.62
			•				27.806	28.277	1.00 16.66
MOTA	90	С	GLY A	69		36.505			
MOTA	91	0	GLY A	69		37.526	28.367	27.771	1.00 15.60
MOTA	92	N	LYS A	70		35.989	26.676	27.804	1.00 17.25
ATOM .	93	CA	LYS A	70		36.556	25.973	. 26.629	1.00 16.95
ATOM	94	C	LYS A	70		35.472	25.138	25.949	1.00 16.87
				70		34.394	24.864	26.562	1.00 17.19
MOTA	95	0	LYS A						1.00 18.62
MOTA	96	CB	LYS A	70		37.737	25.092	27.058	
MOTA	. 97	. CG	LYS A	70		37.518	24.303	28.348	1.00 19.97
MOTA	98	CD	LYS A	70 -		38.737	23.446	28.667	1.00 22.43
ATOM	99	CE	LYS A	70	•	38.538	22.611	29.926	1.00 23.77
MOTA			LYS A	7.0		39.660	21.638	30.129	1.00 22.43
				71		35.714	24.729	24.706	1.00 15.11
ATOM	101	N	SER A				-		1.00 14.34
ATOM	102	CA	SER A	71		34.706	23.950	23.940	
MOTA	103	С	SER A	71	•	34.155	22.730	24.667	1.00 14.36
MOTA	104	0	SER A	71		32.918	22.446	24.600	1.00 13.81
ATOM	105	СВ	SER A	71		35.281	23.523	22.581	1.00 14.97
ATOM	106	0G	SER A	71		36.456	22.743	22.732	1.00 15.41
	-							25.362	1.00 14.38
MOTA	107	N.	GLY A	72		35.024	22.005		
MOTA .	. 108		GLY A	72	•	34.588	20.815	26.072	1.00 14.63
ATOM	109	·C	GLY A	72		33.661	21.022	27.262	1.00 16.49
MOTA	110	0	GLY A	72		32.772	20.159	27.537	1.00 16.20
ATOM	111	N	GLN A	73		33.814	22.129	27.979	1.00 16.78
		CA				32.965	22.369	29.167	1.00 18.67
ATOM:	•								
ATOM .		C	GLN A	73	-	32.040	23.570	29.038	1.00 18.70
MOTA '		,O.,	GLN A	·73		31, 223	23.858	29.967	1.00 19.81
MOTA		CB	GLN A	73		33.852	22.522	30.401	1.00 20.09
ATOM '		·CG	GLN A	73		34.924	21.433	30.493	1.00 24.21
		· CD	GLN A	73		35.624	21.400	31.837	1.00 24.83
ATOM									1.00 26.53
ATOM			GLN A	73		36.048	22.467	32.380	
ATOM	119		GLN A	73		35.769	20.206	32.395	1.00 25.73
MOTA	120	N	GLY A	74		32.138	24.274	27.914	1.00 17.65

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ATOM	121	CA	GLY A	74	31.292	25.429	27.688	1.00 15.83
MOTA	122	С	GLY A	74	31.939	26.746	28.068	1.00 15.56
ATOM	123	0	GLY A	74	32.837	26.799	28.962	1.00 17.53
ATOM	124	N	TYR A	75	31.517	27.814	27.403	1.00 13.96
MOTA	125	CA	TYR A	75	32.041	29.164	27.686	1.00 16.12
ATOM	126	C	TYR A	75	30.991	29.903	28.502	1.00 14.92
MOTA	127	0	TYR A	75	29.758	29.793	28.217	1.00 14.71
\mathtt{ATOM}	128	CB	TYR A	75	32.324	29.918	26.385	1.00 17.79
MOTA	129	CG	TYR A	75	33.490	29.354	25.605	1.00 18.92
ATOM	130	CD1		75	33.326	28.271	24.742	1.00 19.83
MOTA	131	CD2	TYR A	75	34.763	29.909	25.735	1.00 20.43
ATOM	132	CE1	TYR A	75	34.409	27.757	24.020	1.00 21.98
MOTA	133	CE2	TYR A	75	35.847	29.407	25.025	1.00 21.04
ATOM	134	CZ	TYR A	75	35.666	28.339	24.170	1.00 22.04
	135	OH	TYR A	75			23.456	1.00 22.86
ATOM					36.746	27.882		
MOTA	136	N	TYR A	76	31.432	30.653	29.507	1.00 13.66
ATOM	137	CA	TYR A	76	30.478	31.360	30.368	1.00 12.95
ATOM	138	С	TYR A	76	30.753	32.837	30.593	1.00 13.47
ATOM	139	0	TYR A	76	31.901	33.345	30.391	1.00 13.77
				76				1.00 13.77
MOTA	140	CB	TYR A		30.395	30.662	31.725	
ATOM	141	CG	TYR A	76	31.723	30.548	32.446	1.00 14.55
ATOM	142	CD1	TYR A	76	32.601	29.497	32.174	1.00 16.16
MOTA	143	CD2	TYR A	76	32.105	31.495	33.392	1.00 15.68
ATOM	144	CE1	TYR A	76	33.829	29.392	32.832	1.00 17.64
MOTA	145	CE2	TYR A	76	33.329	31.402	34.055	1.00 18.14
ATOM	146	CZ	TYR A	76	34.183	30.348	33.770	1.00 18.24
MOTA	147	OH	TYR A	76	35.390	30.252	34.428	1.00 21.79
ATOM	148	N	VAL A	77	29.716	33.546	31.017	1.00 12.55
ATOM	149	CA	VAL A	77	29.844	34.980	31.298	1.00 14.17
MOTA	150	С	VAL A	77	29.390	35.225	32.727	1.00 15.16
MOTA	151	0	VAL A	7 7	28.564	34.439	33.283	1.00 16.09
ATOM	152	СВ	VAL A	77	28.975	35.821	30.336	1.00 13.43
ATOM	153	CG1	VAL A	77	27.495	35.528	30.567	1.00 11.59
	154	CG2	VAL A	77	29.281			1.00 10.74
ATOM						37.305	30.524	
MOTA	155	N	GLU A	78	29.905	36.276	33.352	1.00 16.88
MOTA	156	CA	GLU A	78	29.486	36.571	34.731	1.00 17.45
MOTA	157	С	GLU A	78	28.178	37.345	34.706	1.00 16.89
ATOM	158	0	GLU A	78	27.961	38.239	33.826	1.00 14.65
	159	СВ	GLU A	78	30.538	37.392	35.479	1.00 19.11
ATOM								
ATOM	160	CG	GLU A	78	30.222	37.503	36.974	1.00 24.70
MOTA	161	CD	GLU A	78	31.225	38.342	37.757	1.00 26.24
MOTA	162	OE1	GLU A	78	31.162	39.584	37.679	1.00 27.53
MOTA	163	OE2	GLU A	78	32.076	37.755	38.452	1.00 29.49
MOTA	164	N	MET A	79	27.296	37.012	35.641	1.00 16.65
MOTA	165	CA	MET A	79	25.992	37.684	35.761	1.00 17.22
\mathtt{MOTA}	166	C	MET A	79	25.610	37.768	37.232	1.00 17.77
ATOM	167	0	MET A	79	26.208	37.066	38.100	1.00 18.29
ATOM	168	CB	MET A	79	24.908	36.899	35.007	1.00 16.88
		CG	MET A			36.874		
ATOM	169			79	25.070		33.492	1.00 16.65
MOTA	170	SD	MET A	79	23.798	35.865	32.673	1.00 17.43
MOTA	171	CE	MET A	79	22.442	37.003	32.577	1.00 15.55
ATOM	172	N	THR A	80	24.637	38.617	37.539	1.00 17.73
ATOM	173	CA	THR A	80				1.00 17.50
					24.146	38.741	38.917	
MOTA	174	C	THR A	80	22.632	38.630	38.853	1.00 17.85
MOTA	175	0	THR A	80	21.995	39.075	37.851	1.00 17.14
MOTA	176	CB	THR A	80	24.524	40.100	39.550	1.00 18.12
ATOM	177	OG1		80	23.851	41.158	38.857	1.00 18.55
MOTA	178	CG2	THR A	80	26.031	40.328	39.474	
								1.00 16.48
ATOM	179	N	VAL A	81	22.042	38.020	39.874	1.00 18.24
ATOM	180	CA	VAL A	81	20.573	37.882	39.959	1.00 20.23
MOTA	181	С	VAL A	81	20.145	38.274	41.375	1.00 21.18
ATOM	182	0	VAL A	81	20.929	38.093	42.362	1.00 20.31
		-			20.525			

MOTA	183	CB	VAL A	81		20.105	36.429	39.700	1.00 20.43
MOTA	184	CG1	VAL A	81		20.566	35.959	38.334	1.00 21.49
MOTA	185	CG2	VAL A	81.		20.639	35.518	40.777	1.00 21.78
MOTA	186	N	GLY A	82		18.938	38.817	41.497	1.00 21.84
ATOM	187		GLY A	82		18.421	39.200	42.799	1.00 21.10
ATOM	188	С	GLY A	82		18.973	40.475	43.404	1.00 21.47
ATOM	189		GLY A	82		19.864	41.159	42.814	1.00 21.97
MOTA	190		SER A	83		18.454	40.808	44.581	1.00 22.27
ATOM	191		SER A	83		18.869	42.012	45.335	1.00 22.02
ATOM	192		SER A	83		18.996	41.607	46.795	1.00 20.16
	193		SER A	83		18.002	41.120	47.410	1.00 20.07
ATOM	193		SER A	83		17.804	43.104	45.213	1.00 20.07
MOTA						17.356	43.229	43.874	1.00 21.30
ATOM	195		SER A	83					1.00 23.70
ATOM	196		PRO A	84		20.198	41.734	47.380	1.00 21.14
MOTA	197		PRO A	84		21.454	42.221	46.785	
MOTA	198		PRO A	84		21.911	41.288	45.656	1.00 20.37
MOTA	199		PRO A	84		21.508	40.086	45.606	1.00 18.46
MOTA	200		PRO A	84		22.434	42.193	47.962	1.00 19.74
ATOM	201		PRO A	84		21.548	42.320	49.166	1.00 20.71
MOTA	202		PRO A	84		20.377	41.447	48.815	1.00 19.44
MOTA	2,03		PRO A	85		22.754	41.790	44.741	1.00 20.53
ATOM	204		PRO A	85		23.258	40.997	43.616	1.00 20.58
ATOM	205	C	PRO A	85		23.949	39.706	44.046	1.00 20.81
MOTA	206		PRO A	85		24.854	39.720	44.936	1.00 21.15
MOTA	207	CB	PRO A	85		24.240	41.947	42.932	1.00 20.87
MOTA	208	CG	PRO A	85		23.732	43.294	43.282	
MOTA	209	CD	PRO A	85		23.340	43.141	44.724	1.00 21.41
MOTA	210	N	GLN A	86		23.541	38.590	43.453	1.00 20.05
MOTA	211	CA	GLN A	86		24.174	37.289	43.752	1.00 19.63
MOTA	212	C T	GLN A	86		24.904	36.923	42.472	1.00 20.50
MOTA	213		GLN A	86		24.263	36.622	41.412	1,00 19.85
MOTA	214		GLN A	86		23.127	36.227	44.097	1.00 19.82
ATOM	215		GLN A			22.283	36.586	45.314	1.00 18.97
ATOM	216		GLN A	86		21.292	35.506	45.693	1.00 19.84
ATOM	217			86		20.226	35.801	46.316	1.00 21.21
ATOM	218			86		21.603	34.259	45.354	1.00 17.54
ATOM	219		THR A	87		26.229	36.969	42.527	1.00 19.61
ATOM	220		THR A	87		27.057	36.669	41.346	1.00 19.61
ATOM	221		THR A	87		27.088	35.188	40.994	1.00 18.63
ATOM	222		THR A	87		27.220	34.302	41.892	1.00 18.56
ATOM	223		THR A	87		28.501	37.164	41.549	1.00 19.88
MOTA	224					28.486	38.558	41.887	1.00 20.57
ATOM	225		THR A			29.304		40.278	1.00 18.65
ATOM	226		LEU A		•	26.972			1.00 18.38
ATOM	. 227		LEU A			26.991	33.522	39.193	1.00 18.18
ATOM	228		LEU A			27.572	33.496		1,00 18.11
MOTA	229		LEU A			27.353	34.457		1.00 18.86
MOTA	230		LEU A		,	25.568	32.952	39.159	1.00 16.21
	231					24.825		40.495	1.00 18.20
MOTA	232		LEU A			23.366		40.226	1.00 18.20
ATOM			LEU A		. *				1.00 16.10
ATOM	233		LEU A			25.484	31.766		
ATOM	234		ASN A			28.317	32.443		1.00 15.84
MOTA	235		ASN A			28.876	32.312	36.101	1.00 16.22
ATOM	236		ASN A		•	27.841	31.544	35.300	1.00 16.03
MOTA	237		ASN A			27.363	30.450	35.735	1.00 15.05
MOTA	238		ASN A			30.208	31.565		1.00 15.71
MOTA	239		ASN A			31.324	32.396	36.700	1.00 16.10
MOTA	240		. ASŅ A			31.390	33.650		1.00 15.48
MOTA	243		ASN A			32.217	31.750		1.00 14.07
MOTA	242	N S	ILE A				32.091		1.00 15.55
MOTA	. 243	CA	ILE A	90			31.494		1.00 14.59
MOTA	24	1 C	ILE A	. 90		26.960	31.052	31.930	1.00 15.07

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MOTA	245	0	ILE A	A	90	27.578	31.867	31.173	1.00 13.01
MOTA	246	СВ	ILE 2	7	90	25.301	32.512	33.084	1.00 14.44
ATOM	247	CG1	ILE A	A.	90	24.884	33.098	34.437	1.00 14.15
ATOM	248	CG2	ILE 2	Δ	90	24.114	31.847	32.407	1.00 14.29
MOTA	249	CD1	ILE A	A.	90	24.356	32.062	35.426	1.00 13.44
MOTA	250	N	LEU A	Α	91	26.714	29.790	31.590	1.00 15.08
ATOM	251	CA	LEU A		91	27.153	29.249	30.284	1.00 15.63
MOTA	252	C	LEU A	A.	91	26.313	29.878	29.174	1.00 16.04
ATOM	253	0	LEU A	λ	91	25.041	29.904	29.250	1.00 16.72
ATOM	254	CB	LEU A	Ą.	91	27.008	27.721	30.265	1.00 14.67
ATOM	255	CG	LEU Z	Α	91	27.450	26.945	29.012	1.00 15.49
	256	CD1	LEU 2		91				
MOTA						27.692	25.485	29.364	1.00 15.10
MOTA	257	CD2	LEU Z	A	91	26.393	27.052	27.925	1.00 15.54
MOTA	258	N	VAL A	Δ	92	26.995	30.408	28.164	1.00 16.13
MOTA	259	CA	VAL A		92	26.336	31.051	27.003	1.00 15.39
MOTA	260	С	VAL A	A	92	25.901	29.960	26.038	1.00 15.51
MOTA	261	0	VAL A		92	26.761	29.243	25.440	1.00 16.92
MOTA	262	CB	VAL A	A.	92	27.306	32.008	26.278	1.00 15.40
MOTA	263	CG1	VAL A	Δ	92	26.668	32.523	24.994	1.00 16.99
MOTA	264	CG2	VAL A		92	27.671	33.172	27.200	1.00 13.64
MOTA	265	N	ASP A	A	93	24.594	29.824	25.845	1.00 16.41
ATOM	266	CA	ASP A	Δ	93	24.069	28.762	24.974	1.00 14.41
MOTA	267	C	ASP A		93	23.090	29.226	23.903	1.00 15.40
ATOM	268	0	ASP A	A.	93	21.889	29.494	24.206	1.00 15.81
	269		ASP A		93				
ATOM		CB				23.411	27.701	25.861	1.00 16.00
ATOM	270	CG	ASP A	Ą	93	22.897	26.512	25.078	1.00 16.45
MOTA	271	OD1	ASP A	Δ	93	23.536	26.133	24.076	1.00 17.23
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MOTA	272	OD2	ASP A		93	21.863	25.938	25.481	1.00 16.68
\mathtt{MOTA}	273	N	THR A	A.	94	23.550	29.326	22.657	1.00 13.38
ATOM	274	CA	THR A	Δ	94	22.636	29.745	21.574	1.00 13.70
MOTA	275	С	THR A	A.	94	21.811	28.549	21.109	1.00 13.68
MOTA	276	0	THR A	A	94	20.941	28.671	20.190	1.00 14.18
ATOM	277	СВ	THR A		94	23.397	30.349	20.362	
ATOM	278	OG1	THR A	A	94	24.279	29.370	19.798	1.00 14.96
ATOM	279	CG2	THR A	A	94	24.201	31.568	20.794	1.00 14.04
ATOM	280	N	GLY A		95	22.053	27.392	21.719	1.00 14.90
\mathtt{ATOM}	281	CA	GLY A	Ą	95	21.309	26.199	21.351	1.00 15.51
ATOM	282	С	GLY A	Δ	95	20.108	25.969	22.255	1.00 16.96
MOTA	283	0	GLY A		95	19.516	24.850	22.275	1.00 16.90
ATOM	284	N	SER A	A	96	19.721	26.987	23.011	1.00 17.38
ATOM	285	CA	SÉR A	2	96	18.562	26.851	23.922	1.00 17.95
MOTA	286	C	SER A	A.	96	17.990	28.231	24.226	1.00 17.07
MOTA	287	0	SER A	Į.	96	18.573	29.269	23.803	1.00 14.94
ATOM	288	CB ·	SER A		96	19.005	26.174	25.219	1.00 18.55
ATOM	289	OG	SER A		96	19.640	26.894	26.276	1.00 26.99
ATOM	290	N	SER A	A.	97	16.869	28.292	24.936	1.00 16.25
ATOM	291	CA	SER A		97				
						16.290	29.614	25.258	1.00 18.39
MOTA	292	С	SER A	J.	97	15.740	29.776	26.670	1.00 17.83
ATOM	293	0	SER A	4	97	14.866	30.653	26.932	1.00 18.75
ATOM	294								
		CB	SER A		97	15.224	29.993	24.227	1.00 18.88
ATOM	295	OG	SER A	7	97	14.633	28.850	23.651	1.00 23.68
MOTA	296	N	ASN A		98	16.229	28.959	27.592	1.00 17.57
MOTA	297	CA	ASN A		98	15.809	29.073	28.993	1.00 16.01
MOTA	298	C	ASN A	Į.	98	16.963	29.611	29.821	1.00 16.51
ATOM	299	0	ASN A		98	18.127	29.109	29.709	1.00 16.69
ATOM	300	CB	ASN A		98	15.401	27.720	29.566	1.00 13.74
ATOM	301	CG	ASN A	A.	98	13.969	27.359	29.241	1.00 16.04
ATOM	302		ASN A		98				
						13.669	26.795	28.139	1.00 13.27
ATOM	303	ND2	ASN A	Ŧ.	98	13.058	27.680	30.158	1.00 13.26
ATOM	304	N	PHE A	Ą	99	16.688	30.640	30.614	1.00 14.45
ATOM	305	CA	PHE A		99				
						17.710	31.196	31.519	1.00 13.19
MOTA	306	С	PHE A	7	99	17.453	30.424	32.812	1.00 13.23

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MOTA	307	0	PHE A 99	16.319	30.466	33.384	1.00 11.00
ATOM	308	CB	PHE A 99	17.491	32.699	31.722	1.00 13.54
MOTA	309	CG	PHE A 99	18.390	33.318	32.761	1.00 14.79
MOTA	310	CD1	PHE A 99.	19.741	32.978	32.836	1.00 15.02
ATOM	311	CD2	PHE A 99	17.889	34.258	33.657	1.00 16.17
MOTA	312	CE1	PHE A 99	20.576	33.564	33.784	1.00 14.99
MOTA	313	CE2	PHE A 99	18.718	34.852	34.610	1.00 16.36
	314	CZ	PHE A 99	20.064	34.503	34.674	1.00 14.33
MOTA				18.457	29.691	33.274	1.00 11.83
ATOM	315	N	ALA A 100	18.298	28.889	34.497	1.00 12.34
MOTA	316	CA	ALA A 100	19.594		35.277	1.00 12.34
MOTA	317	C	ALA A 100		28.836		
ATOM	318	0	ALA A 100	20.722	28.896	34.684	1.00 15.19
ATOM	319	CB	ALA A 100	17.849	27.486	34.138	1.00 13.09
MOTA	320	N	VAL A 101	19.467	28.727	36.595	1.00 13.51
ATOM	321	CA	VAL A 101	20.640	28.686	37.473	1.00 13.80
MOTA	322	С	VAL A 101	20.429	27.693	38.610	1.00 15.86
MOTA	323	O	VAL A 101	19.253	27.424	39.031	1.00 13.90
ATOM	324	CB	VAL A 101	20.912	30.082	38.075	1.00 14:68
MOTA	325		VAL A 101	21.126	31.098	36.962	1.00 12.49
MOTA	326	CG2	VAL A 101	19.743	30.509	38.953	1.00 13.11
ATOM	327	N	GLY A 102	21.528	27.120	39.098	1.00 16.51
MOTA	328	CA	GLY A 102	21.437	26.189	40.207	1.00 17.46
ATOM	329	C	GLY A 102	20.858		41.375	1.00 19.61
MOTA	330	Ö	GLY A 102	21.303	28.128	41.641	1.00 19.12
MOTA	331	N	ALA A 103	19.875	26.395	42.065	1.00 19.81
MOTA	332	CA	ALA A 103	19.241	27.092	43.212	1.00 22.41
MOTA	333	С	ALA A 103	19.098	26.169	44.414	1.00 23.71
MOTA	334	0	ALA A 103	18.196	26.366	45.293	1.00 24.50
MOTA	335	СВ	ALA A 103	17.880	27.627	42.807	1.00 21.12
ATOM	336	N	ALA A 104	19.967	25.168	44.470	1.00 23.53
ATOM	337	CA	ALA A 104	19.979	24.180	45.566	1.00 24.47
ATOM	338	С	ALA A 104	21.341	23.505	45.517	1.00 24.98
ATOM	339	Ö	ALA A 104	21.974	23.413	44.419	1.00 26.65
ATOM	340	СВ	ALA A 104	18.869	23.150	45.367	1.00 23.55
MOTA	341	N	PRO A 105	21.836	23.026	46.668	1.00 25.27
MOTA	342	CA	PRO A 105	23.140	22.361	46.733	1.00 24.87
ATOM	7 3 4 3	C	PRO A 105	23.328	21.286	45.672	1.00 24.16
ATOM	344	0.	PRO A 105	22.350	20.594	45.251	1.00 24.35
MOTA	345	CB	PRO A 105	23.159	21.778	48.143	1.00 25.36
ATOM	346	CG	PRO A 105	22.347	22.763	48.920	1.00 25.71
MOTA	347	CD	PRO A 105	21.183	23.020	47.990	1.00 25.99
MOTA	348	N	HIS A 106	24.566	21.135	45.227	1.00 24.93
ATOM	349	CA	HIS A 106	24.918	20.119		1.00 23.63
MOTA	350	C	HIS A 106	26.402	19.843		1.00 24.29
MOTA	351	0	HIS A 106	27.207			1.00 24.19
MOTA	352	СВ	HIS A 106	24.646	20.622	42.807	1.00 24.15
	353	CG		24.887			1.00 24.43
ATOM ATOM	35 <u>3</u>		HIS A 106 HIS A 106	23.912	19.587 18.702	41.348	1.00 24.43
				26.012		41.084	1.00 23.79
MOTA	355		HIS A 106				1.00 25.66
ATOM			HIS A 106	24.426			1.00 23.00
ATOM	357		HIS A 106	25.699	18.164		1.00 24.92
MOTA	358		PRO A 107		18.572	44.236	
ATOM	359	CA	PRO A 107	28.224	18.200		1.00 26.23
MOTA	360	C	PRO A 107	29.164	19.025	43.474	1.00 26.26
MOTA	361	0	PRO A 107	30.335	19.296		1.00 28.01
MOTA	362	CB	•	28.225	16.722	43.972	1.00 26.21
MOTA	363	CG	PRO A 107	26.875	16.259		
MOTA	364	CD	PRO A 107		17.384		1.00 25.04
ATOM	365	N	PHE A 108	28.695	19.435		1.00 25.94
MOTA	366	CA	PHE A 108	29.556	20.218		1.00 26.76
MOTA	367	C [PHE A 108	29.358	21.726		1.00 26.66
MOTA	368	0	PHE A 108	30.103	22.494	40.778	1.00 26.81

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ATOM	369	CB	PHE A	108	29.368	19.754	39.936	1.00 26.67
ATOM	370	CG	PHE A	108	29.665	18.300	39.720	1.00 26.80
MOTA	371	CD1	PHE A		30.531	17.614	40.569	1.00 27.67
MOTA	372	CD2	PHE A	108	29.090	17.615	38.655	1.00 27.12
ATOM	373	CE1	PHE A	108	30.819	16.262	40.359	1.00 27.99
ATOM	374	CE2	PHE A		29.369	16.267	38.433	1.00 26.65
MOTA	375	CZ	PHE A		30.235	15.587	39.286	1.00 26.94
MOTA	376	N	LEU A	109	28.386	22.180	42.231	1.00 26.14
ATOM	377	CA	LEU A	109	28.144	23.629	42.346	1.00 27.17
ATOM	378	C	LEU A	109	28.914	24.248	43.510	1.00 29.20
ATOM	379	Ö	LEU A		28.861	23.743	44.669	1.00 26.91
MOTA	380	CB	LEU A		26.647	23.911	42.498	1.00 25.73
MOTA	381	CG	LEU A	109	25.811	23.714	41.230	1.00 25.94
ATOM	382	CD1	LEU A	109	24.343	23.983	41.530	1.00 24.99
ATOM	383	CD2	LEU A	109	26.310	24.657	40.136	1.00 24.26
ATOM	384	N	HIS A		29.632	25.328	43.213	1.00 32.94
			HIS A				44.207	
ATOM	385	CA			30.442	26.077		
MOTA	386	С	HIS A		29.533	27.015	44.983	1.00 33.93
ATOM	387	0	HIS A	110	29.732	27.265	46.209	1.00 34.20
MOTA	388	CB	HIS A	110	31.501	26.915	43.485	1.00 42.49
ATOM	389	CG	HIS A	110	32.907	26.469	43.732	1.00 47.84
ATOM	390		HIS A		33.509	26.558	44.969	1.00 50.74
ATOM	391		HIS A		33.834	25.934	42.899	1.00 49.74
ATOM	392		HIS A		34.746	26.098	44.888	1.00 51.83
ATOM	393	NE2	HIS A	110	34.968	25.713	43.644	1.00 51.38
ATOM	394	N	ARG A		28.547	27.553	44.279	1.00 31.13
ATOM	395	CA	ARG A		27.579	28.494	44.857	1.00 28.72
ATOM	396	C	ARG A		26.287	28.331	44.072	1.00 28.16
MOTA	397	0	ARG A		26.267	27.652	43.000	1.00 27.40
MOTA	398	CB	ARG A	111	28.108	29.924	44.717	1.00 28.09
ATOM	399	CG	ARG A	111	28.550	30.255	43.305	1.00 26.48
ATOM	400	CD	ARG A		29.216	31.616	43.201	1.00 25.86
ATOM	401	NE	ARG A		29.723	31.831	41.849	1.00 25.21
MOTA	402	CZ	ARG A		30.423	32.892	41.465	1.00 24.44
MOTA	403	NH1	ARG A	111	30.708	33.850	42.337	1.00 25.08
MOTA	404	NH2	ARG A	111	30.828	32.995	40.205	1.00 22.62
ATOM	405	N	TYR A	112	25.207	28.922	44.566	1.00 26.27
ATOM	406	CA	TYR A	112	23.922	28.814	43.866	1.00 23.70
ATOM	407	C	TYR A		22.955	29.916	44.250	1.00 22.77
MOTA	408	0	TYR A		23.140	30.633	45.283	1.00 21.10
ATOM	409	CB	TYR A	112	23.295	27.437	44.119	1.00 25.47
MOTA	410	CG	TYR A	112	23.036	27.111	45.575	1.00 27.20
MOTA	411	CD1	TYR A	112	21.885	27.569	46.222	1.00 28.51
ATOM	412	CD2			23.946	26.353	46.309	1.00 27.51
ATOM	413		TYR A		21.647	27.276	47.565	1.00 27.78
								1.00 27.78
ATOM	414		TYR A		23.720	26.058	47.651	=
ATOM	415	cz	TYR A	112	22.570	26.522	48.270	1.00 28.98
MOTA	416	OH	TYR A	112	22.352	26.228	49.591	1.00 30.28
ATOM	417	N	TYR A	113	21.927	30.069	43.428	1.00 19.32
ATOM	418	CA	TYR A		20.896	31.090	43.624	1.00 18.94
ATOM		C	TYR A		20.030	30.807		1.00 17.90
							44.857	
ATOM	420	0	TYR A		19.480	29.688	45.011	1.00 19.37
ATOM	421	CB	TYR A	113	20.027	31.141	42.369	1.00 17.76
ATOM	422	CG	TYR A	113	18.887	32.135	42.378	1.00 17.68
ATOM	423		TYR A		19.024	33.397	42.963	1.00 16.86
ATOM	424	CD2			17.709	31.854	41.688	1.00 16.79
ATOM	425		TYR A		18.020		42.848	1.00 17.05
MOTA	426	CE2	TYR A		16.704	32.796	41.563	1.00 16.02
ATOM	427	CZ	TYR A		16.858	34.038	42.138	1.00 17.36
ATOM	428	OH	TYR A	113	15.848	34.963	41.984	1.00 16.62
MOTA	429	N	GLN A		19.967	31.790	45.746	1.00 18.68
ATOM	430	CA	GLN A		19.156	31.673	46.983	1.00 20.28
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ATOM	431	С	GLN A	114		18.057	32.719	46.897	1.00 19.59	
	432	0	GLN A			18.285	33.933	47.192	1.00 20.34	
MOTA						20.028				•
MOTA	433	CB	GLN A				31.912		1.00 19.79	
ATOM	434	CG	GLN A			21.048	30.814	48.434	1.00 22.79	
MOTA	435	CD	GLN A		-	21.942	31.063	49.626	1.00 24.34	
ATOM	436	OE1	GLN A	114		22.708	32.073	49.668	1.00 26.47	
ATOM	437	NE2	GLN A			21.876	30.173	50.606	1.00 24.49	
ATOM	438	N	ARG A			16.876	32.275	46.479	1.00 20.48	
		CA	ARG A			15.703	33.159	46.305	1.00 21.24	
ATOM	439					15.703	33.837	47.583	1.00 21.24	
MOTA	440	C	ARG A							
MOTA	441	0	ARG A			14.784	35.022	47.546	1.00 21.40	
MOTA	442	CB	ARG A	115		14.550	32.366	45.686	1.00 20.21	•
MOTA	443	CG	ARG A	115		14.807	31.953	44.240	1.00 20.95	
ATOM	444	CD	ARG A	115		13.917	30.796	43.824	1.00 20.32	
ATOM	445	NE	ARG A	115		14.305	29.567	44.508	1.00 20.45	
MOTA	446	CZ	ARG A			13.626	28.428	44.448	1.00 19.47	
ATOM	447	NH1	ARG A			12.514	28.352	43.732	1.00 20.02	
ATOM	448		ARG A			14.061	27.366	45.106	1.00 21.63	
								48.710	1.00 22.93	
ATOM	449	N	GLN A			15.323	33.138			
MOTA	450	CA	GLN A			14.880	33.723	49.993	1.00 24.99	
MOTA	451 .	C .	GLN A			15.718	34.953	50.343	1.00 23.86	
MOTA	452	0	GLN A	116		15.242	35.873	51.080	1.00 24.27	
MOTA	453	CB	GLN A	116		14.972	32.691	51.123	1.00 27.81	
MOTA	454	CG	GLN A	116		16.391	32.280	51.502	1.00 32.89	
ATOM	455	CD	GLN A			16.999	31.257	50.550	1.00 36.05	
ATOM	456		GLN A			16.955	31.423	49.295	1.00 36.88	
	457		GLN A			17.577	30.199	51.112	1.00 37.21	
ATOM										
ATOM	458	N	LEU A			16.944	35.006	49.833	1.00 20.91	
MOTA	459	CA	LEU A			17.831	36.153	50.112	1.00 20.59	
MOTA	460	С	LEU A			17.673	37.296	49.124	1.00 19.96	
ATOM	461	0	LEU A	117		18.440	38.301	49.191	1.00 18.93	
MOTA	462	CB	LEU A	117		19.296	35.707	50.128	1.00 21.68	
MOTA	463	CG	LEU A	117		19.887	35:224	51.454	1.00 22.49	
MOTA	464		LEU A	117		19.001	34.175	52.074	1.00 22.63	
ATOM:	465		LEU A			21.286	34.675	51.210	1.00 22.12	
ATOM	466	N	SER A			16.714	37.183	48.210	1.00 18.14	
		CA				16.484	38.252	47.208	1.00 17.08	
ATOM	467		SER A						1.00 17.08	
ATOM	.468	С	SER A			15.150	38.953	47.436		
MOTA	103	0	SER A			14.055	38.316	47.347	1.00 16.00	
MOTA	470	CB	SER A			16.519	37.679 _.	45.787	1.00 15.12	
MOTA .	471	OG	SER A			16.301	38.708	44.835	1.00 16.81	٠
MOTA	472	N	SER A	119		15.210	40.250	47.711	1.00 15.31	
ATOM	473	CA	SER A	119	:	13.991	41.044	47.973	1.00 18.09	
ATOM :		.C	SER A	119		13.169	41.307	46.714	1.00 17.35	
ATOM	475	0	SER A			11.964	41.669	46.800	1.00 17.62	
MOTA	476	CB	SER A			14.371	42.380	48.618	1.00 16.85	
MOTA		OG	SER A			15.158	43.160	47.727	1.00 18.71	
									1.00 18.71	
ATOM .	478	N	THR A			13.781	41.137	45.546		
ATOM	479	CA	THR A			13.075	41.381		1.00 17.26	
MOTA	480	С	THR A			12.587		43.594	1.00 17.17	
ATOM	481	0	THR A	. 120		12.004	40.139	42.466	1.00 18.70	
ATOM	482	CB	THR A	120		13.980	42.143	43.283	1.00 17.78	
MOTA	483	OG1	THR A	120		15.305	41.609	43.355	1.00 17.35	
ATOM .		CG2				14.012	43.630	43.624	1.00 17.37	
ATOM .	485	N	TYR A			12.800	38.977	44.257	1.00 18.03	
MOTA :	486		TYR A			12.364	37.676	43.715	1.00 18.53	
		CA	TYR A		•	10.841		43.713	1.00 18.12	
111 011	487				_		37.584			
MOTA	488	0.	TYR A			10.088	38.028	44.531		
ATOM	489	CB	TYR A		• •	12.878	36.547	44.607	1.00 18.32	
ATOM	490	CG	TYR A			12.187	35.225	44.368	1.00 22.03	
ATOM ·	491	CD1	TYR A	. 121		12.429	34.484	43.209		
ATOM .	492	CD2	TYR A	. 121		11.268	34.725	45.291	1.00 21.95	

MOTA	493	CE1	TYR A	121		11.776	33.280	42.977	1.00 21.33
ATOM	494	CE2	TYR A	121		10.608	33.523	45.067	1.00 22.77
ATOM	495	CZ	TYR A			10.867	32.807		
								43.908	1.00 23.35
MOTA	496	OH	TYR A	121		10.206	31.622	43.682	1.00 23.63
MOTA	497	N	ARG A	122		10.365	37.039	42.492	1.00 16.86
MOTA	498	CA	ARG A	122		8.909	36.851	42.281	1.00 16.79
ATOM	499	C	ARG A			8.703	35.397	41.890	
ATOM	500	0	ARG A			9.348	34.884	40.924	1.00 17.88
ATOM	501	CB	ARG A	122		8.384	37.764	41.174	1.00 14.87
MOTA	502	CG	ARG A	122		8.335	39.230	41.548	1.00 14.83
ATOM	503	CD	ARG A	122		7.895	40.067	40.369	1.00 14.98
ATOM	504	NE	ARG A			7.822	41.481	40.706	1.00 16.19
MOTA	505	CZ	ARG A			7.546	42.442	39.833	1.00 16.67
ATOM	506	NH1	ARG A	122		7.316	42.142	38.559	1.00 15.67
MOTA	507	NH2	ARG A	122		7.505	43.704	40.233	1.00 16.38
MOTA	508	N	ASP A	123		7.836	34.720	42.628	1.00 18.52
ATOM	509	CA	ASP A			7.538	33.296	42.388	1.00 19.00
ATOM	510	C	ASP A			6.435	33.147	41.347	1.00 19.87
ATOM	511	0	ASP A			5.342	33.757	41.490	1.00 17.59
MOTA	512	CB	ASP A			7.090	32.657	43.702	1.00 19.80
ATOM	513	CG	ASP A	123		6.841	31.171	43.582	1.00 20.76
ATOM	514	OD1	ASP A			6.933	30.615	42.463	1.00 20.41
ATOM	515	OD2	ASP A			6.549	30.559	44.629	1.00 22.50
ATOM	516	N	LEU A			6.689	32.359	40.305	1.00 20.70
ATOM	517	CA	LEU A			5.672	32.139	39.255	1.00 21.20
MOTA	518	C	LEU A	124		4.790	30.929	39.562	1.00 21.64
ATOM	519	0	LEU A	124	•	3.832	30.601	38.786	1.00 21.17
ATOM	520	СВ	LEU A	124		6.343	31.978	37.888	1.00 21.51
ATOM	521	CG	LEU A						
						6.850	33.288	37.270	1.00 22.05
MOTA	522	CD1	LEU A			7.617	32.994	35.997	1.00 22.23
MOTA	523	CD2	LEU A	124		5.678	34.217	36.983	1.00 21.49
ATOM	524	N	ARG A	125		5.083	30.252	40.666	1.00 22.67
MOTA	525	CA	ARG A	125		4.286	29.078	41.085	1.00 25.58
MOTA	526	C	ARG A			4.106	28.081	39.944	1.00 26.39
ATOM	527	0	ARG A			2.974	27.552	39.719	1.00 26.83
ATOM	528	CB	ARG A			2.918	29.553	41.593	1.00 26.62
ATOM	529	CG	ARG A			3.016	30.511	42.783	1.00 30.02
ATOM	530	CD	ARG A	125		1.733	31.311	43.002	1.00 32.48
ATOM	531	NE	ARG A	125		1.910	32.334	44.034	1.00 36.63
ATOM	532	CZ	ARG A			1.049	33.323	44.282	1.00 38.12
ATOM	533	NH1	ARG A			-0.070	33.441	43.575	1.00 37.55
MOTA	534	NH2	ARG A			1.307	34.202	45.240	1.00 38.11
MOTA	535	N	LYS A			5189	27.810	39.221	1.00 26.62
MOTA	536	CA	LYS A	126		5.162	26.861	38.079	1.00 26.41
ATOM	537	C	LYS A	126		6.453	26.063	37.986	1.00 24.61
MOTA	538	0	LYS A	126		7.577	26.624	38.141	1.00 22.46
ATOM	539	СВ	LYS A			4.971	27.605	36.756	1.00 28.55
MOTA	540	CG	LYS A			3.539	27.804	36.326	1.00 32.76
ATOM	541	CD	LYS A			3.486	28.380	34.917	1.00 36.53
MOTA	542	CE	LYS A	126		2.048	28.607	34.456	1.00 38.52
ATOM	543	NZ	LYS A	126		1.234	27.355	34.550	1.00 40.78
MOTA	544	N	GLY A			6.326	24.770	37.731	1.00 23.25
ATOM	545	CA	GLY A			7.504			
							23.941	37.598	1.00 22.82
ATOM	546	C	GLY A			7.970	23.995	36.157	1.00 22.77
MOTA	547	0	GLY A			7.220	24.487	35.252	1.00 22.00
ATOM	548	N	VAL A	128		9.184	23.521	35.909	1.00 21.58
MOTA	549	CA	VAL A	128		9.731	23.511	34.541	1.00 22.39
ATOM	550	C	VAL A			10.736	22.388	34.390	1.00 21.31
ATOM	551	0	VAL A			11.547	22.303	35.323	1.00 21.51
ATOM	552	CB	VAL A			10.416	24.851	34.180	1.00 21.77
ATOM	553		VAL A			11.572	25.120	35.122	1.00 22.15
MOTA	554	CG2	VAL A	128		10.903	24.809	32.740	1.00 23.66

ATOM		555	N	TYR A	129			10.700	21.744	33.233	1.00 21.	64
ATOM		556	CA	TYR A				11.598	20.624	32.933	1.00 21.	55
ATOM		557	C	TYR A				12.298	20.882	31.609	1.00 20.3	2.5
MOTA		558	0	TYR A				11.635	21.188	30.573	1.00 20.	
				TYR A				10.785	19.333	32.841	1.00 23.	
MOTA		559	CB									
MOTA		560	CG	TYR A				11.545	18.164	32.271	1.00 26.	
MOTA		561		TYR A				12.628	17.613	32.956	1.00 27.	
MOTA		562	CD2	TYR A				11.178	17.598	31.048	1.00 27.	
MOTA		563	CE1	TYR A	129	•		13.323	16.529	32.443.	1.00 29.	
MOTA		564	CE2	TYR A				11.872	16.507	30.524	1.00 28.	
MOTA		565	CZ	TYR A	129			12.942	15.980	31.231	1.00 28.	91
MOTA		566	OH	TYR A	129			13.634	14.896	30.751	1.00 30.	
MOTA		567	N	VAL A	130			13.620	20.782	31.602	1.00 19.	35
MOTA		568	CA	VAL A	130			14.353	21.003	30.350	1.00 17.	21
ATOM		569	С	VAL A	130			15.308	19.872	30.022	1.00 16.	02
ATOM		570	0	VAL A				16.319	19.628	30.748	1.00 16.	89
ATOM		571	СВ	VAL A				15.136	22.334	30.370	1.00 17.	86
ATOM				VAL A				15.934	22.485	29.075	1.00 15.	31
	.•	573	CG2	VAL A				14.163	23.505	30.525	1.00 15.	
MOTA		574	N.	PRO A				15.013	19.136	28.945	1.00 14.	
ATOM		575	CA	PRO A		•		15.868	18.028	28.529	1.00 14.	
		576	C	PRO A				16.743	18.516	27.372	1.00 15.	
MOTA				PRO A				16.234	19.154	26.402	1.00 15.	
MOTA	,	577	0							28.106	1.00 13.	
ATOM		578	CB.	PRO A				14.857	16.971		1.00 13.	
MOTA		579	CG	PRO A				13.809	17.806	27.421		
MOTA		580	CD	PRO A				13.706	19.078	28.262	1.00 13.	
MOTA		581	N	TYR A				18.043	18.268	27.465	1.00 14.	
MOTA		582	CA	TYR A				18.989		26.404	1.00 17.	
MOTA			. C.	TYR A				19.438	17.415	25.676	1.00 17.	
ATOM	÷	584	0	TYR A				19.100	16.274		1.00 17.	
MOTA		585	CB	TYR A	132			20.211	19.369	27020	1.00 16.	
MOTA		586	CG	TYR A	132			19.909	20.665	27.742	1.00 18.	
MOTA		587	CD1	TYR A	132			19.834	21.881	27.051	1.00 17.	88
MOTA		588	CD2	TYR A	132			19.706	20.681	. 29.122	1.00 19.	01
MOTA		589	CE1	TYR A	132			19.564	23.080	27.722	1.00 16.	57
MOTA	٠.	590	CE2	TYR A	132			19.435	21.867	29.799	1.00 17.	74
MOTA	٠.	591	CZ	TYR A	132			19.365	23.062	29.098	1.00 19.	02
ATOM	•	592	OH	TYR A	132		•	19.083	24.229	29.782	1.00 18.	23
MOTA			N	THR A				20.188	17.574	24.592	1.00 18.	46
ATOM	•	594	CA	THR A				20.686	16.403	23.842	1.00 18.	54
ATOM	٠.		C	THR A		-		21.525	15.580	24.812	1.00 20.	42
MOTA		596		THR A					14.325	24.672		
ATOM				THR A				21.546		22.653	1.00 18.	
ATOM				THR A				20.720	17.539		1.00 20.	
ATOM				THR A				22.194	15.645		1.00 18.	
ATOM		600	N	GLN A				22.064	16.265		1.00 22.	
ATOM				GLN A				22.890	15.624		1.00 24.	
MOTA		602	C	GLN A				22.723	16.406		1.00 23.	
		603	0:	GLN A				23.179		28.252		
ATOM											1.00 21.	
MOTA			CB	GLN A				24.352	15.633		• •	
MOTA				GLN A				25.140	14.412		1.00 32.	
ATOM			CD	GLN A				25.020	13.296		1.00 36.	
MOTA		607		GLN A				26.052	12.680		1.00 37	
MOTA				GLN A			٠	23.791	13.018		1.00 38.	
MOTA			N	GLY F				22.080	15.789		1.00 23.	
ATOM		610	CA	GLY A				21.863	16.460	30.391	1.00 21.	
ATOM			C.	GLY F				20.432	16.946	30.483	1.00 22.	
MOTA		612	0	GLY F					17.111		1.00 20.	
MOTA				LYS P	•			19.968			•	
ATOM			CA	LYS A				18.584		31.923	1.00 23.	
ATOM	· _	615	C.	LYS A				18.429	18.147	33.353	1.00 22.	
MOTA	,	616	0 -	LYS F	136			19.196	17.719	34.269	1.00 21.	42

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MOTA	617	CB	LYS	Α	136	17.606	16.501	31.677	1.00 25.37
ATOM	618	CG	LYS	Δ	136	17.823	15.310	32.607	1.00 28.29
ATOM	619								
		CD	LYS			16.804	14.196	32.374	1.00 31.54
ATOM	620	CE	LYS	Α	136	16.955	13.570	31.000	1.00 34.21
ATOM	621	NZ	LYS	Α	136	15.996	12.444	30.789	1.00 37.76
ATOM	622	N			137		19.040		
						17.470		33.573	1.00 21.02
ATOM	623	CA	TRP	Α	137	17.214	19.562	34.928	1.00 20.75
ATOM	624	С	TRP	Α	137	15.750	19.907	35.133	1.00 20.62
ATOM	625	Ō	TRP			14.951	19.978		
								34.153	1.00 20.05
MOTA	626	CB	TRP	А	137	18.077	20.800	35.231	1.00 18.46
MOTA	627	CG	TRP	Α	137	17.960	21.937	34.248	1.00 18.02
ATOM	628	CD1	TRP	Δ	137	18.865	22.276	33.281	1.00 18.12
					-				
MOTA	629	CD2			137	16.881	22.879	34.134	1.00 17.27
MOTA	630	NE1	TRP	Α	137	18.419	23.369	32.574	1.00 17.78
MOTA	631	CE2	TRP	Α	137	17.204	23.758	33.074	1.00 17.40
MOTA	632	CE3			137	15.675	23.067		
								34.823	1.00 17.08
ATOM	633	CZ2			137	16.363	24.807	32.684	1.00 15.50
ATOM	634	CZ3	TRP	А	137	14.836	24.113	34.434	1.00 17.23
MOTA	635	CH2	TRP	A	137	15.188	24.968	33.373	1.00 17.46
ATOM	636	N	GLU						
						15.385	20.098	36.395	1.00 21.53
MOTA	637	CA	${ t GLU}$	А	138	14.014	20.472	36.789	1.00 24.94
ATOM	638	С	GLU	A	138	14.166	21.642	37.745	1.00 23.18
ATOM	639	0	GLU			15.168	21.719		1.00 21.21
								38.526	
MOTA	640	CB	GLU		138	13.320	19.320	37.515	1.00 28.46
ATOM	641	CG	${ t GLU}$	Α	138	13.053	18.101	36.656	1.00 34.91
ATOM	642	CD	GLU	А	138	12.562	16.919	37.472	1.00 37.93
ATOM	643	OE1				12.175			
							15.897	36.864	1.00 40.28
MOTA	644	OE2	GLU	А	138	12.570	17.009	38.722	1.00 40.20
ATOM	645	N	GLY	А	139	13.214	22.559	37.711	1.00 22.13
MOTA	646	CA	GLY	Δ	139	13.298	23.693	38.604	1.00 22.60
ATOM	647	С	GLY			11.975	24.402	38.713	1.00 21.54
ATOM	648	0	GLY	Α	139	10.949	23.953	38.116	1.00 23.29
ATOM	649	N	GLÜ	Α	140	11.962	25.494	39.465	1.00 21.74
ATOM	650	CA	GLU						
						10.733	26.284	39.648	1.00 21.81
ATOM	651	С	${ t GLU}$	A	140	10.900	27.646	38.998	1.00 19.04
ATOM	652	0	GLU	Α	140	11.975	28.304	39.125	1.00 18.42
ATOM	653	CB	GLU	Δ	140	10.404	26.425	41.139	1.00 24.39
ATOM	654	CG	GLU			11.479	25.887	42.065	1.00 28.61
MOTA	655	CD	GLU	Α	140	10.922	25.385	43.383	1.00 29.72
ATOM	656	OE1	GLU	A	140	10.311	24.297	43.389	1.00 31.43
ATOM	657	OE2	GLU		140	11.091	26.077	44.410	
									1.00 30.48
MOTA	658	N	LEU			9.870	28.071	38.278	1.00 16.35
ATOM	659	CA	LEU	A	141	9.901	29.360	37.585	1.00 15.48
ATOM	660	С	LEU	Α	141	9.674	30.546	38.511	1.00 15.68
ATOM	661	Ó	LEU			8.832			
							30.499	39.466	1.00 13.45
MOTA	662	CB ·				8.864	29.376	36.460	1.00 15.23
MOTA	663	CG	LEU	Α	141	9.145	28.412	35.300	1.00 16.27
MOTA	664	CD1	LEU .	Α	141	8.008	28.461	34.300	1.00 15.60
ATOM	665		LEU .						
						10.458	28.785	34.627	1.00 16.48
ATOM	666	N	GLY .			10.424	31.608	38.241	1.00 15.15
ATOM	667	CA	GLY .	Α	142	10.323	32.819	39.015	1.00 12.33
ATOM	668	С	GLY .			10.845	33.953		
								38.167	1.00 14.67
MOTA	669	0	GLY .			11.242	33.758	36.971	1.00 13.75
ATOM	670	N	THR .	A	143	10.877	35.137	38.754	1.00 14.88
ATOM	671	CA	THR .	A	143	11.354	36.324	38.050	1.00 15.26
ATOM	672	C	THR .						
						12.262	37.103	39.008	1.00 14.53
ATOM	673	0	THR .			12.119	36.991	40.269	1.00 13.46
ATOM	674	CB	THR .	A	143	10.131	37.154	37.600	1.00 16.18
ATOM	675	OG1				10.192	37.362	36.187	1.00 20.69
ATOM	676	CG2	THR .						
						10.058	38.465	38.325	1.00 12.43
ATOM	677	N	ASP :			13.202	37.866	38.466	1.00 14.22
ATOM	678	CA	ASP A	A	144	14.117	38.652	39.321	1.00 15.38
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MOTA		679	С	ASP A	144	•	14.942	39.609	38.479	1.00 15.67
ATOM		680	Ō	ASP A			14.984	39.496	37.208	1.00 16.83
							15.063	37.721	40.086	1.00 15.20
MOTA		681	СВ	ASP A		-				
MOTA		682	CG	ASP A			15.367	38.218	41.496	1.00 17.84
MOTA	•	683	OD1	ASP A	144		15.359	39.447	41.724	1.00 16.62
ATOM	٠	684	OD2	ASP A	144		15.630	37.373	42.379	1.00 16.33
		685	N	LEU A			15.596	40.551	39.147	1.00 16.74
MOTA										
MOTA		686	CA	LEU A			16.442	41.537	38.454	1.00 18.66
ATOM		687	C	LEU A	145		17.757	40.854	38.101	1.00 20.21
MOTA		688	0	LEU A	145		18.381	40.147	38.961	1.00 21.75
ATOM		689	СВ	LEU A	145	•	16.697	42.746	39.351	1.00 18.43
			CG	LEU A			15.452	43.522	39.786	1.00 19.69
MOTA		690					15.878	44.720	40.628	1.00 19.11
ATOM		691		LEU A						
MOTA		692	CD2	LEU A			14.660	43.971	38.557	1.00 18.50
MOTA		693	N	VAL A	146		18.186	41.030	36.858	1.00 20.48
ATOM		694	CA	VAL A	146		19.426	40.402	36.387	1.00 21.21
ATOM		695	C	VAL A			20.331	41.426	35.725	1.00 22.80
				VAL A			19.849	42.386	35.045	1.00 22.16
MOTA		696 .	0.						35.373	1.00 20.39
MOTA		697	СВ	VAL A		•	19.118	39.265		
MOTA		698	CG1	VAL A	146	•	20.405	38.575	34.941	1.00 20.39
ATOM		699	.CG2	VAL A	146		18.163	38.261	35.998	1.00 17.90
ATOM	. •	700	N	SER A	147		21.633	41.251	35.913	1.00 22.35
ATOM		701	CA	SER A			22.615	42.158	35.309	1.00 23.39
				SER A			23.829	41.383	34.833	1.00 21.77
MOTA		702	C							
MOTA	•	703	0	SER A			24.119	40.242	35.321	1.00 20.08
MOTA		704	CB	SER A	147		23.059	43.225	36.316	1.00 25.41
MOTA		705	OG	SER A	147		21.993	44.107	36.627	1.00 31.97
MOTA		706	N	ILE A	148		24.534	41.972	33.878	1.00 19.69
ATOM		707	CA	ILE A			25.757	41.377	33.329	1.00 19.14
										1.00 18.85
MOTA		708	C	ILE A			26.853	42.405	33.614	
MOTA		709	0	ILE A			27.021	43.408	32.853	1.00 17.87
MOTA	•	710	CB	ILE A	148		25.618	41.137	31.817	1.00 18.61
MOTA		711	CG1	ILE A	148		24.449	40.181	31.559	1.00 19.01
ATOM		712	CG2				26.909	40.564	31.255	1.00 17.68
							24.221	39.864	30.097	1.00 19.61
MOTA		713	CD1							
MOTA		714	N	PRO A			27.601	42.214	34.711	1.00 17.99
MOTA	:	. 715	CA	PRO A	149		28.679	43.134	35.095	1.00 21.17
MOTA	• .	.716	C.	PRO A	149		29.523	43.638	33.926	1.00 22.18
ATOM		717	0	PRO A	149		29.800	44.869	33.823	1.00 24.08
ATOM	•	718	СВ	PRO A			29.485	42.317	36.103	1.00 19.87
ATOM	,	719	CG	PRO A		_	28.404	41.529	36.797	1.00 19.57
										1.00 17.55
MOTA		720	CD	PRO A			27.542	41.061	35.628	
MOTA		721	N	HIS A			29.930	42.733	33.041	1.00 23.43
MOTA	**	722	CA	HIS A	150		30.748	43.119	31.869	1.00 23.84
MOTA	-	723	С	HIS A	150		29.933	43.067	30.588	1.00 24.47
ATOM		724	0	HIS A			30.334	42.431	29.566	1.00 25.89
				HIS A				42.211	31.765	1.00 23.54
ATOM		725				-				
ATOM		726	CG	HIS A			32.880	42.313	32.945	1.00 26.15
MOTA	•	727		HIS A			33.619	43.446		1.00 27.28
MOTA		728	CD2	HIS A	150	•	33.149	41.439	33.943	1.00 26.32
ATOM		729	CE1	HIS A	150		34.305	43.264	34.330	1.00 27.48
ATOM	:			HIS A			34.038	42.055	34.791	1.00 28.01
								43.727	30.630	1.00 25.49
MOTA			N.	GLY A			28.785			
MOTA	• •	732	CA	GLY A			2.7.906	43.784	29.485	1.00 26.41
MOTA		733	С	GLY A	151		27.325	45.179	29.468	1.00 27.16
ATOM	•	734	0	GLY A	151		27.981	46.136	29.983	1.00 26.97
MOTA	•	735	N	PRO A			26.125	45.370	28.903	1.00 28.12
	٠.	736	CA	PRO 7			25.540		28.880	1.00 28.75
ATOM							• '			1.00 20.73
MOTA	•		C	PRO A			25.219		30.304	
MOTA		738	Ö	PRO A			24.844	46.331	31.182	1.00 28.62
MOTA	٠.	739	ĊВ	PRO A	152		24.294	46.528	28.017	1.00 29.49
MOTA		740	CG	PRO A	152	•	23.897	45.105	28.303	1.00 29.85
								•		

ATOM	741	CD	PRO A	152		25.227	44.385	28.277	1.00 28.15
ATOM	742	N	ASN A			25.375	48.457	30.560	1.00 28.13
ATOM	743	CA	ASN A			25.373	49.016		
MOTA	744	C	ASN A					31.902	1.00 34.39
MOTA	745	0	ASN A			23.604	49.096	32.144	1.00 33.81
						23.009	50.218	32.222	1.00 33.63
ATOM	746	CB	ASN A			25.755	50.401	32.009	1.00 37.16
ATOM	747	CG	ASN A			25.680	50.978	33.406	1.00 38.88
MOTA	748		ASN A			25.974	50.272	34.416	1.00 40.17
MOTA	749	ND2				25.309	52.251	33.504	1.00 39.91
MOTA	750	И	VAL A			22.971	47.934	32265	1.00 31.55
MOTA	751	CA	VAL A			21.514	47.872	32.486	1.00 29.59
MOTA	752	С	VAL A	_		21.113	46.739	33.418	1.00 29.47
MOTA	753	0	VAL A			21.924	45.809	33.718	1.00 30.24
ATOM	754	CB	VAL A			20.755	47.681	31.154	1.00 29.95
MOTA	755	CG1		154		20.990	48.875	30.242	1.00 29.70
MOTA	756	CG2	VAL A	154		21.216	46.397	30.474	1.00 28.94
MOTA	75 7	N	THR A	155		19.874	46.799	33.882	1.00 27.83
ATOM	758	CA	THR A	155		19.323	45.773	34.779	1.00 27.61
ATOM	759	С	THR A	155		17.918	45.472	34.296	1.00 26.01
ATOM	760	. 0	THR A	155		17.114	46.413	34.041	1.00 27.70
ATOM	761	CB	THR A	155		19.268	46.280	36.229	1.00 27.24
MOTA	. 762	OG1	THR A	155		20.603	46.486	36.703	1.00 29.54
MOTA	763	CG2	THR A	155		18.573	45.270	37.129	1.00 27.37
MOTA	764	N	VAL A	156		17.592	44.197	34.143	1.00 24.69
ATOM	765	CA	VAL A	156		16.241	43.847	33.672	1.00 24.32
MOTA	766	С	VAL A	156		15.631	42.736	34.504	1.00 23.23
ATOM	767	0	VAL A	156		16.364	41.920	35.154	1.00 23.57
ATOM	· 768	CB	VAL A	156		16.253	43.402	32.184	1.00 25.34
MOTA	769	CG1	VAL A	156		17.178	44.302	31,379	1.00 26.63
MOTA	770	CG2	VAL A	156		16.684	41.960	32.063	1.00 24.89
ATOM	771	N .	ARG A	157		14.306	42.687	34.521	1.00 21.44
MOTA	772	CA	ARG A	157		13.613	41.626	35.262	1.00 20.90
MOTA	773	С	ARG A	157	• •	13.374	40.560	34.215	1.00 20.13
ATOM	774	0	ARG A	1.5.7		12.746	40.836	33.152	1.00 19.99
MOTA	775	CB	ARG A	157		12.280	42.121	35.830	1.00 20.03
ATOM	776	CG	ARG A	157		11.528	41.053	36.621	1.00 18.95
MOTA	777	CD	ARG A	157		10.271	41.616	37.260	1.00 18.99
ATOM	778	NE	ARG A	157		10.554	42.408	38.456	1.00 18.47
MOTA	779	cz	ARG A	157		10.973	41.902	39.613	1.00 19.19
MOTA	780	NH1	ARG A	157		11.167	40.596	39.747	1.00 18.30
ATOM	781	NH2	ARG A	157		11.178	42.703	40.650	1.00 15.82
MOTA	782	N	ALA A	158		13.878	39.359	34.463	1.00 20.27
ATOM	783	CA	ALA A	158		13.713	38.266	33.496	1.00 19.08
MOTA	784	C	ALA A			13.279	36.986	34.175	1.00 19.45
MOTA	785	0	ALA A	158		13.379	36.845	35.432	1.00 19.64
MOTA	786	CB	ALA A	158		15.017	38.031	32.756	1.00 18.56
ATOM	787	N	ASN A	159		12.792	36.053	33.370	1.00 18.08
ATOM	788	CA	ASN A	159		12.363	34.756	33.876	1.00 18.21
ATOM	789	C	ASN A	159		13.607	33.992	34.282	1.00 18.60
ATOM	790	0	ASN A	159		14.666	34.033	33.577	1.00 19.42
ATOM	791	CB	ASN A	159		11.601	33.992	32.797	1.00 16.91
MOTA	792	CG	ASN A			10.282	34.647	32.459	1.00 18.46
MOTA	793		ASN A			9.479	34.978	33.381	1.00 19.46
MOTA	794		ASN A	159		10.020	34.848	31.174	1.00 16.51
ATOM	795	N	ILE A	160		13.518	33.311	35.412	1.00 18.73
ATOM	796	CA	ILE A			14.643	32.529	35.916	1.00 17.64
MOTA	797	С	ILE A			14.112	31.191	36.373	1.00 19.09
ATOM	798	0	ILE A			13.122	31.125	37.176	1.00 18.38
ATOM	799	CB	ILE A			15.319	33.212	37.128	1.00 18.36
ATOM	800	CG1	ILE A			15.764	34.629	36.758	1.00 17.90
MOTA	801	CG2	ILE A			16.521	32.394	37,585	1.00 17.16
MOTA	802	CD1	ILE A	160		16.521	35.336	37.875	1.00 18.56

ATOM		803	N	ALA A	161	14.717	30.123	35.871	1.00 17.55
ATOM		804	CA		161	14.314	28.778	36.275	1.00 18.11
ATOM		805	C	ALA A	161	15.267	28.394	37.399	1.00 18.26
		806	0	ALA A		16.507	28.223	37.166	1.00 17.61
MOTA									
MOTA		807	СВ	ALA A		14.447	27.805	35.105	1.00 17.28
ATOM		808	N	ALA A		14.737	28.283	38.614	1.00 17.99
MOTA		809	CA	ALA A		15.567	27.901	39.775	1.00 18.02
MOTA		810	C	ALA A	162	15.746	26.382	39.774	1.00 18.52
ATOM		811	0	ALA A		14.835	25.619	40.207	1.00 18.43
MOTA		812	CB	ALA A		14.897	28.359	41.067	1.00 17.36
ATOM		813	N	ILE A	163.	16.900	25.928	39.300	1.00 19.89
MOTA		814	CA	ILE A	163	17.204	24.480	39.215	1.00 18.56
MOTA		815	С	ILE A	163	17.314	23.802	40.577	1.00 20.34
MOTA		816	0	ILE A	163	18.238	24.122	41.402	1.00 19.83
MOTA		817	CB	ILE A	163	18.512	24.245	38.430	1.00 17.19
MOTA		818	CG1	ILE A		18.347	24.753	36.994	1.00 16.02
ATOM		819	CG2	ILE A		18.874	22.761	38.445	1.00 14.93
ATOM		820	CD1	ILE A		19.628	24.735	36.174	1.00 16.24
ATOM		821	N	THR A		16.409	22.860	40.826	1.00 20.42
MOTA		822	CA	THR A		16.379	22.122	42.112	1.00 23.01
MOTA		823	C	THR A		16.817	20.665	41.958	1.00 24.30
		824	0	THR A		17.119	19.966	42.973	1.00 26.25
MOTA								_	
MOTA		825	CB	THR A		14.966	22.173	42.735	
MOTA		826	OG1	THR A		13.990	21.799	41.754	1.00 22.15
MOTA		827	CG2	THR A	164	14.656	23.584	43.214	1.00 22.73
MOTA		828 .		GLU. A	165	16.858	20.187	40.721	1.00 25.84
MOTA		829	CA	GLU. A		17.281	18.804	40.444	1.00 27.82
MOTA		830	C	GLU A		17.800	18.693	39.024	1.00 26.80
MOTA		831	0	GLU. A		17.246	19.323	38.072	1.00 26.59
MOTA	•	832	CB	GLU A	165	16.121	17.834	40.678	1.00 31.67
MOTA	•	833	СĠ	GLU A	165	16.233	17.118	42.020	1.00 38.94
ATOM		834	CD.	GLU A	165	14.913	16.568	42.519	1.00 41.54
ATOM		835	OE1	GLU A	165	14.282.	15.765	41.796	1.00 44.35
MOTA		836	OE2	GLU A	165	14.510	16.940	43.644	1.00 43.84
ATOM		837	N	SER A	166	18.861	17.919	38.852	1.00 24.81
MOTA		838	CA	SER A	166.	19.455	17.765	37.525	1.00 25.32
MOTA		839	С.	SER A	166	20.213 .		37.397	1.00 25.44
ATOM	:	840	0	SER A		20:.551	15.795	38.427	1.00 24:00
ATOM		841	CB	SER A		20.405	18.928	37.255	1.00 2313
ATOM		842	OG	SER A			18.939	38.217	1.00 21.22
ATOM		843	N.	ASP A		20.490.	16.079	36.155	1.00 26.01
ATOM		844	CA	ASP A		21.227		35.871	
MOTA		845	C	ASP A		22.138		34.671	1.00 25.62
ATOM		846	0.	ASP. A		21.656		33.528	1.00 24.35
ATOM			CB	ASP A		20.253	13.691	35.601	1.00 30.53
MOTA		848	CG	ASP A		20.255		35.387	1.00 30.33
									1.00 32.07
MOTA		850		ASP A		21.912 . 20.586		36.152	
MOTA								34.469	
ATOM		851	N.	LYS A		23.440		34.910	1.00 25.32
MOTA			CA.		168	24.461			1.00 25.94
MOTA	•				168	24.416.		33.175	1.00 25.49
MOTA				LYS A		24.742	16.580	31.955	1.00 25.50
MOTA		855	CB	LYS A		24.282:		32.800	1.00 27.68
MOTA			CG	LYS A		24.408	12.570.		1.00 30.33
MOTA	-		CD	LYS A		24.117	11.532	32.292	1.00 32.36
MOTA	£		CE	LYS. A	.168	24.205	10.126	32.855	1.00 34.37
MOTA		859	NZ	LYS. A	168	23.889	9.101	31.821	1.00 36.50
MOTA		. 860	И.	PHE A	169	24.024	17.460	33.937	1.00 22.87
MOTA		.861	CA	PHE A	169.	23.942		33.418	1.00 20.96
MOTA	٠	862	C	PHE A			19.616		1.00 22.06
MOTA	٠		Ο.	PHE A		25.983			1.00 20.71
MOTA	•	864	CB	PHE A			19.506	33.919	1.00 19.76

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MOTA

926

CE3 TRP A 176

25.635 33.918

1.00 18.29

26.852

MOTA	927	CZ2	TRP	A	176			27.794	23	. 532	32.252	1.00	17.40
ATOM	928	CZ3	TRP	Α	176.		- ;	26.034		. 557	33.573	1.00	19.02
MOTA	929	CH2	TRP	Α	176			26.512		.521	32.747	1.00	19.06
ATOM	930	N .						27.496		.950	37.005	1.00	18.68
MOTA	931	CA	GLU					26.387		. 385	37.797		21.01
MOTA	932	C	GLU					25.024		.700	37.224		20.81
ATOM	933	0	GLU					23.977		.582	37.938		21.08
MOTA	934	CB	GLU					26.461		.869	39.250		22.84
ATOM	935	CG	GLÜ					26.865		.322	39.443		26.63
ATOM	936	CD	GLU					28.377		.531	39.446		27.90
	937		GLU					29.121		.568	39.726		28.44
ATOM	938		GLU					28.818		. 670	39.186		28.24
MOTA	939	N	GLY					25.010		.088	35.953		18.48
MOTA MOTA	940	CA	GLY					23.759		.411	35.295		16.82
	941	CA	GLY					23.739		.406	33.791		15.90
MOTA	941		GLY					25.070		.248	33.264		15.75
MOTA	943	0	ILE			•		22.831		.589	33.076		14.53
MOTA		N	ILE					22.831		.588	31.610		14.26
MOTA	944	CA C	ILE			•		22.007		.701	31.010		14.53
ATOM	945 946		ILE					20.896		.980	31.603		15.23
ATOM		0 .						20.830		.217	31.069		14.45
MOTA	947	CB	ILE							.183	29.548		14.28
ATOM	948	CG1 CG2						22.535		.921	31.525		13.41
ATOM	949		ILE					21.002 22.359		.788	28.974		13.41
MOTA	950 051	CD1								. 350	29.998		14.91
ATOM	951	N	LEU					22.489			29.353		14.24
ATOM	952	CA	LEU.					21.763		.464	27.961		15.19
MOTA	953 054	C	LEU					21.311		.050	26.973		15.79
MOTA	954	0			180			22.117		.115			14.83
MOTA	955	CB	LEU					22.675		.690 .			16.59
MOTA	956	CG	LEU					22.078		.107 .996	29.257 28.351		15.04
MOTA	957		LEU					22.902					17.08
MOTA	· 958		LEU			•		20.622		.120 .621	28.818 27.851		15.40
MOTA	959	N	GLY					20.057		. 227			13.68
MOTA	960	CA	GLY					19.525			26.561		15.03
MOTA	961	C	GLY					19.276 18.402		.481	25.741 26.107		14.58
MOTA	962	0	GLY							.330 .629	24.638		12.84
ATOM	963	N						20.002					13.53
MOTA	964	CA	LEU					19.859 - 19.029		.646	23.787 22.521	• •	14.25
MOTA	•	O .	LEU		182			18.883		.607	21.701		13.52
MOTA	966 967	CB	LEU					21.250		.352	23.418		13.44
MOTA	968							22.036		.949	24.583		11.84
MOTA MOTA	969	CG	LEU		182			23.506					11.17
	970	CDI	LEU	Α.	102	-		21.450			24.936		12.14
MOTA	971	N N	אד.א	λ·	102			18.491		.449	22.322		15.12
ATOM	972	CA			183			17.660		.183	21.131		15.16
~ ~~~	077	C	מו.מ	ν.	103			16.276	31	.788	21.361		17.66
MOTA	074	Ö.	7T.7	y W	103			16.278		.526	22.377		16.26
MOTA	974			_				17.557		.684	20.875		14.23
	976	N	WAR	Α.	101			15.338			20.873		18.41
MOTA			TIL	Α.	104	•							17.40
ATOM ATOM	977	CA			184			13.976		.060	20.550		18.41
	978	C.	TIK	A	104 104	-		12.953		.334	21.424 21.807		14.95
MOTA	979	0			184			13.131		.135			18.07
MOTA	980	CB			184	-		13.411		.237	19.138		
ATOM	981	CG			184			14.327		.017	18.216		19.50
MOTA	982		TYR					15.295		.367	17.446		19.23 19.65
ATOM	983		TYR					14.233		.408	18.119		19.03
MOTA	. 984		TYR	A	104	1		16.144 15079		.083	16.599	•	
MOTA	985	CE2	T.XK	A	184.					.134			19.50
ATOM	986	CZ						16.027		.466	16.521		19.86 20.69
ATOM	987	OH	TXK	A	184			16.842			15.670		16.29
MOTA	988	N	ALA	А	TR2	٠.		11.873	32	.046	21.734	1.00	10.43

						_			
MOTA	989	CA	ALA A	. 185	10.784	31.519	22.592	1.00	17.90
ATOM	990	С	ALA A	185	10.185	30.221	22.068	1 00	17.38
MOTA	991	0	ALA A		9.682	29.372		1.00	15.41
MOTA	992	CB	ALA A	185	9.690	32.579	22.742	1.00	15.99
MOTA	993	N	GLU A						
					10.232	30.046	20.751		20.56
ATOM	994	CA	GLU A	186	9.679	28.846	20.086	1.00	23.43
ATOM	995	С	GLU A	186	10.169	27.533	20.690		23.87
ATOM	996	0	GLU A	T86	9.448	26.486	20.619	1.00	24.67
ATOM	997	CB	GLU A	186	10.009	28.887	18.591	1.00	27.60
ATOM	998	CG	GLU A						
-					9.447	27.729	17.786		32.42
ATOM	999	CD	GLU A	186	7.941	27.593	17.923	1.00	36.08
MOTA	1000	OE1	GLU A	186	7.255	28.633	18.041	1 00	39.03
ATOM		OE2							
	1001				7.439	26.448	17.900	1.00	37.05
ATOM	1002	N	ILE A	187	11.363	27.540	21.283	1.00	22.31
MOTA	1003	CA	ILE A	187	11.904	26.302	21.900		19.35
MOTA	1004	С	ILE A	187	12.113	26.441	23.403	1.00	20.13
MOTA	1005	0	ILE A	187	12.887	25.654	24.034	1.00	19.35
MOTA	1006	СВ	ILE A		13.241	25.872	21.248	1.00	
ATOM	1007	CG1			14.270	26.998	21.355	1.00	18.36
ATOM	1008	CG2	ILE A	187	13.008	25.488	19.795	1 00	19.03
MOTA	1009	CD1				26.635			
					15.627		20.780		17.45
ATOM	1010	N	ALA A	188	11.441	27.416	23.999	1.00	19.82
ATOM	1011	CA	ALA A	188	11.551	27.636	25.454	1.00	20.35
MOTA	1012								
		С	ALA A		10.622	26.661	26.171		19.60
ATOM	1013	0	ALA A	188	9.554	26.277	25.618	1.00	19.52
ATOM	1014	CB	ALA A	188	11.160	29.083	25.793		17.16
ATOM									
	1015	N	ARG A		11.004	26.231	27.372		20.77
\mathtt{MOTA}	1016	CA	ARG A	189	10.142	25.324	28.164	1.00	21.43
ATOM	1017	С	ARG A	189	9.577	26.162	29.303		22.80
MOTA	1018	0	ARG A	189	10.274	27.099	29.817	1.00	23.68
MOTA	1019	CB	ARG A	189	10.949	24.151	28.753	1.00	22.36
ATOM	1020	CG	ARG A	189	11.689	23.285	27.729		
									23.90
MOTA	1021	CD	ARG A	189	10.765	22.818	26.624	1.00	24.33
MOTA	1022	NE	ARG A	189	11.419	21.914	25.681	1.00	25.35
MOTA	1023	CZ	ARG A		11.336				
						20.586	25.724		27.35
MOTA	1024	NH1	ARG A	189	10.620	19.991	26.673	1.00	24.73
ATOM	1025	NH2	ARG A	189	11.959	19.849	24.807	1.00	25.42
MOTA	1026	N	PRO A		8.325				
						25.890	29.725		23.27
ATOM	1027	CA	PRO A	190	7.442	24.830	29.216	1.00	23.21
ATOM	1028	С	PRO A	190	6.826	25.110	27.849		23.72
MOTA	1029	0	PRO A						
					6.458	24.157	27.101		23.77
ATOM	1030	CB	PRO A	190	6.377	24.713	30.305	1.00	22.63
ATOM	1031	CG	PRO A	190	6.285	26.115	30.830		24.33
ATOM	1032								
		CD	PRO A		7.745	26.527	30.921		22.73
MOTA	1033	N	ASP A		6.681	26.383	27.508	1.00	25.20
ATOM	1034	CA	ASP A	191	6.107	26.754	26.202	1 00	25.89
ATOM	1035	C	ASP A						
					6.653	28.106	25.770	1.00	25.76
MOTA	1036	0	ASP A	191	7.488	28.716	26.498	1.00	24.40
MOTA	1037	СВ	ASP A	191	4.569	26.757	26.269		28.36
ATOM									
	1038	CG	ASP A		4.024	27.697	27.323	1.00	30.16
ATOM	1039	OD1	ASP A	191	2.887	27.468	27.783	1.00	33.88
ATOM	1040		ASP A		4.714	28.669	27.686		30.53
MOTA	1041	N	ASP A		6.214	28.596	24.617	1.00	26.01
MOTA	1042	CA	ASP A	192	6.724	29.877	24.088	1.00	26.22
MOTA	1043	C	ASP A						
					6.236	31.123	24.813		26.52
MOTA	1044	Ó	ASP A		6.567	32.275	24.395	1.00	26.27
MOTA	1045	CB	ASP A	192	6.419	29.985	22.589		27.69
MOTA	1046	CG	ASP A						
					4.940	30.161	22.296		29.61
MOTA	1047	OD1	ASP A		4.102	29.647	23.066	1.00	31.87
MOTA	1048	OD2	ASP A	192	4.618	30.805	21.279	1.00	30.31
ATOM	1049	N	SER A						
					5.470	30.947	25.885		24.46
MOTA	1050	CA	SER A	193	4.988	32.117	26.645	1.00	24.21

MOTA	1051	С	SER A	193		6.078	32.565	27.614	1.00 22.68
MOTA	1052	Ö	SER A			6.082	33.740	28.082	1.00 22.41
						3.701	31.787		
MOTA	1053	CB	SER A					27.415	
MOTA	1054	OG	SER A			3.910	30.774	28.386	1.00 27.13
ATOM	1055	N	LEU A	194		7.009	31.670	27.932	1.00 20.84
ATOM	1056	CA	LEU A	194		8.107	32.044	28.852	1.00 18.87
MOTA	1057	C	LEU A			9.149	32.830	28.065	1.00 18.82
	1058		LEU A			10.066	32.240	27.419	1.00 19.19
MOTA		0							
MOTA	1059	CB	LEU A			8.758	30.809	29.469	1.00 17.48
MOTA	1060	CG	LEU A			9.680	31.201	30.631	1.00 19.18
MOTA	1061	CD1	LEU A	194		8.825	31.633	31.825	1.00 16.80
MOTA	1062	CD2	LEU A	194		10.585	30.044	31.014	1.00 16.32
MOTA	1063	N	GLU A	195		9.025	34.150	28.095	1.00 18.44
ATOM	1064	CA	GLU A			9.949	35.029	27.369	1.00 18.80
MOTA	1065	C	GLU A			11.415	34.777	27.733	1.00 19.02
						11.791	34.754	28.953	1.00 17.72
MOTA	1066	.0	GLU A						
MOTA	1067	CB	GLU A			9.575	36.485	27.644	1.00 20.83
ATOM	1068	CG	GLU A			10.514	37.512	27.047	1.00 23.03
ATOM ·	1069	CD	GLU A	195		9.989	38.926	27.204	1.00 24.10
ATOM	1070	OE1	GLU A	195		9.211	39.373	26.337	1.00 25.77
ATOM	1071	OE2	GLU A	195		10.343	39.585	28.203	1.00 24.06
MOTA	1072	N	PRO A			.12.272	34.559	26.714	1.00 18.43
MOTA	1073	CA		196		13.702	34.311	26.935	1.00 18.17
	1073	C	PRO A			14.385	35.571	27.447	1.00 16.90
ATOM									
MOTA	1075	0	PRO A			13.845	36.715	27.297	1.00 17.67
ATOM '	1076	. CB	PRO A			14.210	33.914	25.546	1.00 17.79
MOTA	1077	CG	PRO A	196		12.992	33.305	24.892	1.00 19.11
MOTA	1078	CD	PRO A	196		11.911	34.287	25.310	1.00 18.58
ATOM	1079	N	PHE A	197		15.558	35.405	28.039	1.00 15.80
ATOM	1080	CA	PHE A			16.290	36.550	28.574	1.00 14.47
ATOM	1081	C	PHE A			16.597	37.663	27.576	1.00 16.31
MOTA	1082	0	PHE A			16.392	38.873	27.894	1.00 14.87
			PHE A					29.217	1.00 12.99
ATOM	1083	CB				17.595	36.093		
MOTA	1084	CG		197		18.472	37.227	29.652	1.00 13.09
MOTA	1085	CD1				19.376	37.806	28.767	1.00 12.33
ATOM	1086	CD2	PHE A	197		18.347	37.766	30.926	1.00 14.29
MOTA	1087	CE1	PHE A	197		20.139	38.907	29.143	1.00 12.22
MOTA	1088	CE2	PHE A	197		19.108	38.873	31.310	1.00 14.64
ATOM	1089	CZ	PHE A	197		20.002	39.441	30.415	1.00 13.26
ATOM	1090		PHE A			17.089	37.319	26.390	1.00 16.71
MOTA	1091	CA	PHE A			17:427	38.384	25.431	1.00 17.60
								25.001	1.00 17.52
MOTA	1092	C	PHE A			16.212	39.192		
MOTA	1093	0	PHE A			16.317	40.434	24.774	1.00 16.03
MOTA	1094	CB	PHE A			18.133	37.829	24.196	1.00 17.77
MOTA	1095	CG	PHE A			19.051	38.826	23.549	1.00 17.92
MOTA	1096	CD1	PHE A	198		20.310	39.075	24.087	1.00 18.66
MOTA	1097	CD2	PHE A	198		18.633	39.569	22.455	1.00 16.90
ATOM	1098	CE1	PHE A	198		21.139	40.053	23.546	1.00 18.55
ATOM	1099		PHE A		,	19.454	40.551	21.904	1.00 17.96
ATOM	1100	CZ	PHE A			20.708	40.795	22.451	1.00 18.52
MOTA	1101	N	ASP A					24.879	1.00 17.52
						15.066	38.530		
ATOM	1102	CA	ASP A			13.819	39.225	24.491	1.00 19.54
MOTA	1103	С	ASP A			13.464	40.261	25.561	1.00 18.83
MOTA	1104	. 0	ASP A			13.134	41.444	25.233	1.00 20.48
MOTA	1105	CB	ASP A	199		12.685	38.210	24.338	1.00 21.95
MOTA	1106	CG	ASP A	199		12.868	37.312	23.126	1.00 24.77
ATOM	1107		ASP A			12.408	37.687	22.028	1.00 27.27
ATOM	1108		ASP A			13.481	36.234	23.261	1.00.27.11
ATOM	1109	N	SER A			13.530	39.858	26.829	1.00 17.89
MOTA		CA							1.00 17.83
	1110		SER A			13.223	40.784	27.947	
MOTA	1111	C,	SER A			14.211	41.943	27.915	1.00 16.77
MOTA	1112	Ο.	SER A	200		13.823	43.140	28.072	1.00 17.20

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MOTA	1113	CB	SER A	200	13.336	40.062	29.292	1.00 14.55
MOTA	1114	OG	SER A	200	12.386	39.017	29.400	1.00 14.16
MOTA	1115	N	LEU A	201	15.481	41.617	27.711	1.00 16.47
ATOM	1116	CA	LEU A	201	16.553	42.638	27.654	1.00 18.93
MOTA	1117	С	LEU A	201	16.237	43.684	26.586	1.00 18.88
ATOM	1118	0	LEU A		16.274	44.917	26.852	1.00 18.26
ATOM	1119	CB	LEU A		17.884	41.953	27.337	1.00 18.68
ATOM	1120	CG	LEU A		19.244	42.637	27.523	1.00 20.59
ATOM	1121	CD1			19.973	. 42.616	26.194	1.00 20.98
ATOM	1122	CD2	LEU A		19.100	44.053	28.045	1.00 20.13
ATOM	1123	N	VAL A		15.919	43.222	25.383	1.00 20.38
ATOM	1124	CA	VAL A		15.600	44.130	24.264	1.00 20.33
ATOM	1125	C	VAL A		14.335	44.938	24.532	1.00 20.23
ATOM	1126	0	VAL A		14.284	46.175	24.255	1.00 23.15
ATOM	1127	CB	VAL A		15.433	43.337	22.948	1.00 23.30
ATOM	1128	CG1	VAL A		14.830	44.228	21.855	1.00 19.84
ATOM	1129	CG1	VAL A		16.792	42.804	22.502	1.00 17.80
	1130	N N	LYS A		13.315		25.074	
ATOM					12.050	44.285		1.00 24.15
ATOM	1131	CA	LYS A			44.985	25.360	1.00 27.77
ATOM	1132	C	LYS A		12.178	46.049	26.452	1.00 27.47
ATOM	1133	0	LYS A		11.753	47.223	26.252	1.00 26.63
MOTA	1134	CB	LYS A		10.970	43.973	25.746	1.00 29.55
ATOM	1135	CG	LYS A		9.609	44.594	26.008	1.00 34.08
ATOM	1136	CD	LYS A		8.497	43.798	25.335	1.00 36.82
ATOM	1137	CE	LYS A		8.504	42.342	25.774	1.00 38.97
ATOM	1138	NZ	LYS A		7.512	41.533	25.012	1.00 40.86
ATOM	1139	N	GLN A		12.771	45.687	27.585	1.00 26.46
ATOM	1140	CA	GLN A		12.910	46.632	28.721	1.00 26.94
ATOM	1141	C	GLN A		14.125	47.542	28.614	1.00 28.51
ATOM	1142	0	GLN A		14.479	48.264	29.600	1.00 30.36
MOTA	1143	CB	GLN A		13.007	45.848	30.032	1.00 24.17
ATOM	1144	CG	GLN A		11.980	44.739	30.170	1.00 20.78
MOTA	1145	CD	GLN A		12.270	43.821	31.342	1.00 20.14
ATOM	1146	OE1	GLN A		11.725	42.676	31.420	1.00 19.72
MOTA	1147	NE2	GLN A		13.107	44.279	32.265	1.00 16.56
ATOM	1148	N	THR A		14.762	47.568	27.453	1.00 28.58
ATOM	1149	CA	THR A		15.979	48.375	27.306	1.00 29.06
ATOM	1150	C	THR A		16.186	48.905	25.885	1.00 30.58
ATOM	1151	0	THR A		15.427	48.525	24.940	1.00 30.23
ATOM	1152	CB	THR A		17.175	47.501	27.772	1.00 29.85
ATOM	1153	OG1	THR A		17.572	47.899	29.088	1.00 29.62
ATOM	1154	CG2	THR A		18.328	47.576	26.823	1.00 29.03
ATOM	1155	N	HIS A		17.175	49.784	25.711	1.00 31.92
ATOM	1156	CA	HIS A		17.488	50.350	24.372	1.00 33.38
ATOM	1157	C	HIS A		18.548	49.530	23.637	1.00 32.31
MOTA	1158	0	HIS A		18.905	49.845	22.460	1.00 31.08
MOTA	1159	CB	HIS A		17.975	51.799	24.487	1.00 36.39
ATOM	1160	CG	HIS A		16.898	52.773	24.848	1.00 39.92
ATOM	1161		HIS A		15.696	52.836	24.177	1.00 40.95
ATOM	1162	CD2	HIS A		16.849	53.736	25.800	1.00 40.35
MOTA	1163		HIS A		14.951	53.794	24.699	1.00 41.58
ATOM	1164	NE2	HIS A		15.627	54.356	25.685	1.00 41.65
ATOM	1165	N	VAL A		19.075	48.501	24.291	1.00 29.55
MOTA	1166	CA	VAL A		20.097	47.639	23.651	1.00 28.49
ATOM	1167	C	VAL A		19.511	47.083	22.354	1.00 26.27
ATOM	1168	0	VAL A		18.415	46.441	22.358	1.00 26.26
ATOM	1169	CB	VAL A		20.498	46.462	24.572	1.00 28.77
ATOM	1170	CG1			21.399	45.491	23.825	1.00 29.45
ATOM	1171	CG2	VAL A		21.219	46.987	25.805	1.00 28.52
ATOM	1172	N	PRO A		20.192	47.311	21.220	1.00 24.42
ATOM	1173	CA	PRO A		19.683	46.804	19.944	1.00 23.82
ATOM	1174	С	PRO A	208	19.547	45.284	19.914	1.00 22.81

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A	MOT	1175	0	PRO A	A 208		20.290	44.545	20.630	1.00 21.12	
	TOM	1176	CB	PRO A	A 208		20.689	47.343	18.926	1.00 24.65	
	MOT	1177	CG	PRO Z	A 208		21.927	47.510	19.711	1.00 25.77	
	MOT	1178	CD	PRO Z	A 208		21.441	48.062	21.025	1.00 24.39	
	TOM	1179	N		A 209		18.605	44.806	19.109	1.00 21.59	
	TOM	1180	CA		A 209		18.322	43.362	18.995	1.00 20.43	
	TOM	1181	C		A 209		19.390	42.599	18.222	1.00 20.52	
	TOM	1182	Ö		A 209		19.190	42.217	17.026	1.00 21.39	
	TOM	1183	СВ		A 209		16.957	43.159	18.340	1.00 18.52	
	TOM	1184	CG		A 209		16.501	41.728	18.402	1.00 18.12	
	TOM	1185			A 209		16.968	40.948	19.281	1.00 18.32	
	TOM	1186			A 209		15.594	41.348	17513	1.00 15.63	
	TOM	1187	N		A 210		20.514	42.346	18.883	1.00 19.53	
	TOM	1188	CA		A 210		21.631	41.634	18.243	1.00 19.83	
	TOM	1189	C		A 210		22.765	41.421	19.226	1.00 19.02	
	TOM	1190	0		A 210		22.958	42.238	20.176	1.00 18.52	
	TOM	1191	СВ		A 210		22.120	42.451	17.035	1.00 21.93	
	TOM	1192	CG		A 210		23.534	42.305	16.456	1.00 22.75	
	TOM	1193			A 210		23.612	43.009	15.102	1.00 23.20	
	TOM	1194			A 210		24.548	42.910	17.409	1.00 24.60	
	TOM	1195	N		A 211		23.509	40.334	19.044	1.00 16.48	
	TOM	1196	CA		A 211		24:671	40.055	19.909	1.00 16.70	
	TOM	1197	C		A 211		25.722	39.310	19.095	1.00 16.08	
	TOM	1198	Õ		A 211		25.392		18.063	1.00 17.22	
	TOM	1199	СВ		A 211		24.251	39.280	21.173	1.00 14.67	
	TOM	1200	CG		A 211		23.813	37.863	20.924	1.00 16.01	
	MOT	1201	CD1		A 211		24.748	36.837	20.835	1.00 14.91	
	TOM	1202			A 211		22.465	37.546	20.824	1.00 14.62	2
	MOT	1203			A 211		24.344	35.515	20.653	1.00 15.05	5
	MOT	1204			A 211		22.054	36.224	20.641	1.00 15.47	7
	MOT	1205	CZ		A 211		22.996	35.207	20.558	1.00 12.73	3 .
	MOTA	1206	N		A 212		26.977	39.424	19.520	1.00 17.19	•
	MOT	1207	CA		A 212		28.126	38.803	18.818	1.00 16.98	3
	MOTA	1208	Ċ		A 212	-	28.894	37.862	19.725	1.00 16.10)
	TOM	1209	0		A 212		29.036	38.122	20.955	1.00 14.22	2
	MOTA	1210	CB	SER	A 212		29.094	39.888	18.349	1.00 16.89	€
	MOTA	1211	OG	SER	A 212		28.431	40.869	17.593	1.00 26.70) .
	MOTA	1212	N	LEU	A 213		29.430	36.797	19.144	1.00 14.76	5
	· MOTA	1213	CA		A 213		30.194	35.819	19.930	1.00 14.81	L.
	MOTA	1214	С	LEU	A 213		31.563	35.509	19.352	1.00 14.32	
7	MOTA	1215	0	LEU	A 213		31.702	35.162	18.137	1.00 12.74	1.
P	MOTA	1216	СВ	LEU	A 213		29.394	34.522	20.060	1.00 15.67	7 .
	MOTA	1217	CG	LEU	A 213		28.735	34.210	21.408	1.00.18.95	5
P	MOTA	1218	CD1	LEU	A 213		28.196	35.475	22.050	1.00 18.65	5
7	· MOTA	1219	CD2	LEU	A 213		27.627	33.185	21.192	1.00 16.46	5
Į	MOTA	1220	N	GLN	A 214		32.581	35.656	20.191	1.00 14.19	€
Į	MOTA	. 1221	CA	GLN	A 214		33.954	35.324	19.797	1.00 15.89	9
Į	MOTA	1222	С	GLN	A 214		34.407	34.258	20.778	1.00 15.04	4.
Į	MOTA	1223	0	GLN	A 214		34.848	34.582	21.917	1.00 16.01	1
I	MOTA	1224	СВ	GLN	A 214		34.903	36.523	19.914	1.00 17.92	
I	MOTA	1225	CG	GLN	A 214	•	36.290	36.231	19.341	1.00 20.63	3
7	MOTA	1226	CD	GLN	A 214		37.397	37.099	19.932	1.00 23.22	2
	MOTA	1227			A 214		38.459	37.332	19.273	1.00 24.79	
7	MOTA	1228	NE2	GLN	A 214		37.199	37.571	21.156	1.00 24.53	
7	MOTA	1229	N	LEU	A 215		34.284	32.997	20.390	1.00 14.3	
	MOTA	1230	CA		A 21,5		34.729	31.890	. 21.262	1.00 13.74	4
	MOTA	1231	·C		A 215		36.193	31.625	20.925	1.00 14.40	
	· MOTA	1232	0		A 215		36.541	31.357	19.737	1.00 14.39	9
	MOTA	1233	CB		A 215		33.872	30.644	21.005	1.00 13.9	4 .
2	MOTA	1234	CG		A 215		32.636	30.429	21.893	1.00 14.78	
	MOTA	1235		LEU	À 215		31.900	31.734	22.143	1.00 13.3	1 .
	MOTA		· CD2	LEU	A 215		31.723	29.407	21.240	1.00 12.9	7
								•			

MOTA	1237	N	CYS	A 216	37.066	31.706	21.922	1.00 14.	. 83
ATOM	1238	CA	CVS	A 216	38.504	31.486	21.682	1.00 16.	
MOTA	1239	С		A 216	39.066	30.196	22.263	1.00 17	. 20
MOTA	1240	0	CYS	A 216	39.174	30.046	23.519	1.00 16.	.79
MOTA	1241	CB		A 216	39.314	32.668	22.227	1.00 19	
MOTA	1242	SG	CYS	A 216	38.852	34.278	21.505	1.00 23	.75
MOTA	1243	N	GLY	A 217	39.415	29.257	21.387	1.00 15	. 43
MOTA	1244	CA		A 217	40.018	28.021	21.843	1.00 16	
MOTA	1245	С	GLY	A 217	41.483	28.371	22.064	1.00 17.	. 87
ATOM	1246	0	GLY	A 217	42.057	29.204	21.303	1.00 17.	. 53
ATOM	1247	N		A 218	42.119	27.785	23.069	1.00 17	
ATOM	1248	CA	ALA	A 218	43.539	28.108	23.349	1.00 16	. 33
ATOM	1249	С	ALA	A 218	44.486	27.408	22.379	1.00 17.	.71
ATOM	1250	0	ΔΤ.Δ	A 218	45.602	27.927	22.069	1.00 16.	46
ATOM	1251	CB		A 218	43.884	27.731	24.779	1.00 14	
ATOM	1252	N	${ t GLY}$	A 219	44.073	26.245	21.890	1.00 16.	. 19
ATOM	1253	CA	GLY	A 219	44.909	25.505	20.970	1.00 17	57
ATOM	1254	C		A 219	45.696	24.439	21.703	1.00 17	
MOTA	1255	0	\mathtt{GLY}	A 219	46.490	23.675	21.076	1.00 16.	. 29
MOTA	1256	N	PHE	A 220	45.502	24.375	23.018	1.00 17.	.13
ATOM	1257	CA		A 220	46.190	23.381	23.873	1.00 18.	
MOTA	1258	С		A 220	45.381	23.185	25.153	1.00 19.	. 24
ATOM	1259	0	PHE	A 220	44.477	24.012	25.475	1.00 19.	. 69
MOTA	1260	CB		A 220	47.616	23.854	24.187	1.00 18.	
MOTA	1261	CG		A 220	47.689	25.253	24.731	1.00 20.	. 0 /
ATOM	1262	CD1	PHE	A 220	47.448	25.507	26.077	1.00 20.	.91
ATOM	1263	CD2	PHE	A 220	47.984	26.320	23.890	1.00 19.	91
MOTA	1264	CE1		A 220	47.505	26.809	26.576	1.00 21.	
ATOM	1265	CE2	PHE	A 220	48.043	27.620	24.374	1.00 20.	. 35
ATOM	1266	CZ	PHE	A 220	47.802	27.866	25.721	1.00 21.	77
ATOM	1267	N		A 221	45.659	22.110	25.907		
								1.00 20.	
ATOM	1268	CA	PRO	A 221	44.922	21.846	27.147	1.00 21.	. 27
ATOM	1269	С	PRO	A 221	45.014	22.959	28.180	1.00 23.	.04
MOTA	1270	0		A 221	46.065	23.666	28.292	1.00 23.	
ATOM	1271	CB		A 221	45.545	20.543	27.648	1.00 20.	. 22
ATOM	1272	CG	PRO	A 221	45.946	19.855	26.390	1.00 20.	. 63
ATOM	1273	CD	PRO	A 221	46.571	20.994	25.602	1.00 20.	45
				A 222					
MOTA	1274	N			43.934	23.132	28.933	1.00 25.	
\mathtt{ATOM}	1275	CA	LEU	A 222	43.873	24.158	29.991	1.00 28.	. 32
MOTA	1276	С	LEU	A 222	43.425	23.516	31.291	1.00 30.	88
ATOM	1277	0		A 222	42.248	23.042	31.403	1.00 31.	
ATOM	1278	CB	LEU	A 222	42.880	25.261	29.620	1.00 27.	
MOTA	1279	CG	LEU	A 222	43.264	26.233	28.506	1.00 27.	.30
MOTA	1280	CD1	LEU	A 222	42.040	27.042	28.096	1.00 26.	
				A 222					
ATOM	1281				44.382	27.143	28.983	1.00 27.	
MOTA	1282	N	ASN	A 223	44.320	23.470	32.273	1.00 34.	. 15
ATOM	1283	CA	ASN	A 223	43.959	22.893	33.583	1.00 37.	64
ATOM		C		A 223					
	1284				43.014	23.882	34.254	1.00 38.	
ATOM	1285	0	ASN	A 223	42.864	25.056	33.785	1.00 36.	72
MOTA	1286	CB	ASN	A 223	45.204	22.663	34.457	1.00 38.	54
ATOM	1287	CG		A 223	45.905	23.952	34.839	1.00 39.	
MOTA	1288			A 223	45.268	24.903	35.375	1.00 41.	
ATOM	1289	ND2	ASN	A 223	47.208	24.013	34.595	1.00 40.	09
ATOM	1290	N		A 224	42.380	23.444	35.335	1.00 41.	
MOTA	1291	CA		A 224	41.415	24.278	36.073	1.00 43.	
ATOM	1292	С	GLN	A 224	41.898	25.708	36.359	1.00 42.	52
MOTA	1293	0	GLN	A 224	41.138	26.705	36.126	1.00 42.	
ATOM	1294	CB		A 224	41.021	23.572	37.378		
								1.00 46.	
MOTA	1295	CG		A 224	39.629	23.956	37.827	1.00 49.	86
MOTA	1296	CD	GLN	A 224	39.085	23.160	38.990	1.00 51.	40
ATOM	1297	OE1		A 224	37.923	23.406	39.443	1.00 52.	
ATOM	1298	NE2	אונדט	A 224	39.866	22.215	39.496	1.00 52.	/5

MOTA	1299	N	SER A	225		43.133	25.852	36.831	1.00 40.27
ATOM	1300	CA	SER A			43.669	27.200	37.138	1.00 39.30
	1300	CA	SER A			43.989	28.028	35.893	1.00 36.57
MOTA			SER A			43.920	29.292	35.930	1.00 36.27
ATOM	1302	0				44.917	27.094	38.027	1.00 40.27
MOTA	1303	CB	SER A						1.00 40.27
MOTA	1304	OG	SER A			45.974	26.411	37.376	
MOTA	1305	N	GLU A			44.339	27.364	34.796	1.00 34.29
MOTA	1306	CA	GLU A			44.654	28.083	33.542	1.00 32.79
MOTA	1307	С	GLU A			43.375	28.651	32.954	1.00 31.17
MOTA	1308	0	GLU A			43.354	29.815	32.454	1.00 29.09
MOTA	1309	CB	GLU A			45.307	27.144	32.526	1.00 33.69
MOTA	1310	CG	GLU A			46.708	26.696	32.902	1.00 36.40
MOTA	1311	CD	GLU A			47.251	25.619	31.972	1.00 37.70
MOTA	1312	OE1	GLU A	226		46.585	24.567	31.830	1.00 37.54
MOTA	1313	OE2	GLU A	226		48.340	25.823	31.389	1.00 37.14
MOTA	1314	N	VAL A	227		42.305	27.867.	33,007	1.00 29.89
MOTA	1315	CA	VAL A	227		41.013	28.312	32.458	1.00 30.15
MOTA	1316	С	VAL A	227		40.512	29.547	33.203	1.00 29.84
ATOM	1317	0	VAL A	227		39.922	30.484	32.582	1.00 30.30
MOTA		CB	VAL A			39.940	27.210	32.558	1.00 30.93
ATOM	1319	CG1	VAL A			38.800	27.538	31.637	1.00 32.67
ATOM	1320		VAL A			40.516	25.867	32.183	1.00 32.31
ATOM	1321	N	LEU A			40.731	29.581	34.513	1.00 28.88
ATOM	1322	CA	LEU A			40.292	30.726	35.336	1.00 27.31
ATOM	1323	C	LEU A			41:059	31.992	34.975	1.00 27.59
MOTA	1324	Õ	LEU A			40.491	33.129	35.020	1.00 27.84
ATOM	1325	CB	LEU F			40.496	30.420	36.819	1.00 27.50
ATOM	1326	CG	LEU F			39.700	29.259	37.419	1.00 29.32
ATOM	1327		LEU A			40.129		38.867	1.00 28.16
MOTA	1328		LEU A		•	38.205	29.549	37.339	1.00 28.58
ATOM	1329	N N	ALA A			42.327	31.835	34.610	1.00 27.12
	1330	CA	ALA A			43.176	32.998	34.257	1.00 27.64
MOTA	1331	CA	ALA A			43.176	33.347	32.776	1.00 27.65
MOTA			ALA A			43.460	34.504	32.776	1.00 27.03
MOTA	1332	0				44.617		34.682	1.00 27.52
MOTA	1333	CB	ALA A			42.736	32.736 32.393	31.947	1.00 27.52
ATOM	1334	N		230				30.498	1.00 26.33
MOTA	1335	CA		4 230 4 230		42.692	32.635	30.438	1.00 26.22
	1336	C				41.438	33.360	30.695	1.00 25.70
ATOM	1337	0		A 230		40.356	33.302	29.746	1.00 25.70
ATOM	1338	CB		A 230		42.815	31.310 31.519	28.344	1.00 26.54
ATOM	1339	OG		A 230		42.759			1.00 25.03
MOTA	1:340	N	VAL A			41.562	34.056		
MOTA	1341	CA		A 231	•	40.415	34.764.		1.00 24.89 1.00 24.75
ATOM	1342	C		A 231		39.785	33.776		
MOTA	1343	0		A 231		40.453	33.310	26.371	1.00 25.97
MOTA	1344	CB		A 231		40.859	36.043	27.568	1.00 24.38
ATOM	1345		VAL A			39.729	36.554		1.00 22.98
MOTA	1346		VAL 2			41.244	37.119		1.00 23.20
ATOM	1347			A 232		38.526	33.433		1.00 23.26
MOTA	1348	CA		A 232		37.846	32.481	26.729	•
MOTA	1349		GLY A			37.125	33.081	25.538	1.00 21.57
MOTA	1350	0		A 232		36.590	32.324	24.666	1.00 20.69
MOTA	1351	N		A 233		37.078	34.408	25.468	1.00 19.21
ATOM	1352	CA		A 233		36.410	35.050	24.353	1.00 17.96
ATOM	1353	С		A 233		35.599		24.731	1.00 18.25
ATOM	1354	0		A 233		35.778		25.851	1.00 15.19
MOTA	1355	N		A 234		34.7.08	36.677	23.828	1.00 16.58
ATOM ·		CA		A 234		33.864	37.864	24.053	
ATOM	1357	C.		A 234		32.423			·
ATOM.	1358	0		A 234			36.995		
MOTA	1359	·СВ		A 234		34.426	39.072		
MOTA	1360	OG	SER A	A 234	• .	35.816	39.253	23.508	1.00 18.23

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ATOM	1361	N	MET A	235	31.506	38.227	24.372	1.00 18.00
	1362	CA	MET A		30.091	38.201	24.010	1.00 17.58
ATOM								
MOTA	1363	С	MET A	235	29.732	39.677	23.996	1.00 18.27
ATOM	1364	0	MET A	235	29.594	40.322	25.087	1.00 19.03
						37.475		
MOTA	1365	CB		235	29.232		25.046	1.00 16.91
MOTA	1366	CG	MET A	235	27.759	37.455	24.634	1.00 17.60
ATOM	1367	SD	MET A	235	26.597	36.751	25.819	1.00 20.56
MOTA	1368	CE		235	25.105	36.803	24.857	1.00 21.69
ATOM	1369	N	ILE A	236	29.629	40.248	22.801	1.00 19.70
MOTA	1370	CA	ILE A	236	29.271	41.669	22.674	1.00 19.40
MOTA	1371	С	ILE A		27.764	41.758	22.522	1.00 20.06
ATOM	1372	0	ILE A	236	27.175	41.365	21.467	1.00 16.87
ATOM	1373	СВ	ILE A	236	29.985	42.341	21.470	1.00 21.41
ATOM	1374	CG1	ILE A		31.452	42.625	21.821	1.00 22.57
MOTA	1375	CG2	ILE A	236	29.329	43.672	21.149	1.00 21.72
ATOM	1376	CD1	ILE A	236	32.243	41.426	22.228	1.00 25.65
ATOM	1377	N	ILE A	237	27.122	42.246	23.575	1.00 20.16
MOTA	1378	CA	ILE A		25.663	42.382	23.599	1.00 21.01
ATOM	1379	С	ILE A	237	25.215	43.710	22.996	1.00 22.16
MOTA	1380	0	ILE A	237	25.620	44.812	23.472	1.00 22.96
			ILE A				25.050	1.00 21.36
MOTA	1381	СВ			25.153	42.241		and the second s
MOTA	1382	CG1	ILE A	237	25.346	40.791	25.498	1.00 22.29
ATOM	1383	CG2	ILE A	237	23.694	42.660	25.156	1.00 20.45
ATOM	1384	CD1	ILE A		25.002	40.529	26.939	1.00 24.84
MOTA	1385	N	GLY A	238	24.404	43.626	21.946	1.00 23.30
ATOM	1386	CA	GLY A	238	23.903	44.820	21.288	1.00 25.11
ATOM	1387	С	GLY A	238	24.821	45.437	20.244	1.00 26.35
MOTA	1388	0	GLY A		24.644	46.640	19.874	1.00 27.08
ATOM	1389	N	GLY A	239	25.792	44.681	19.743	1.00 25.50
MOTA	1390	CA	GLY A	239	26.679	45.251	18.747	1.00 24.81
ATOM	1391	C	GLY A		27.807	44.371	18.242	1.00 26.38
MOTA	1392	0	GLY A	239	27.942	43.167	18.632	1.00 23.61
ATOM	1393	N	ILE A	240	28.632	44.960	17.383	1.00 26.33
ATOM	1394	CA	ILE A	240	29.780	44.273	16.758	1.00 25.87
MOTA	13,95	С	ILE A		31.067	45.033	17.055	1.00 26.95
ATOM	1396	0	ILE A	240	31.121	46.287	16.882	1.00 28.86
ATOM	1397	CB	ILE A	240	29.607	44.226	15.226	1.00 25.88
ATOM	1398	CG1	ILE A	240	28.298	43.519	14.871	1.00 25.12
ATOM	1399	CG2	ILE A		30.806	43.541	14.581	1.00 26.56
ATOM	1400	CD1	ILE A	240	27.939	43.599	13.396	1.00 24.59
ATOM	1401	N	ASP A	241	32.100	44.323	17.498	1.00 25.24
MOTA	1402	CA	ASP A		33.395	44.973	17.781	1.00 25.13
ATOM	1403	С	ASP A	241	34.383	44.548	16.698	1.00 26.31
MOTA	1404	0	ASP A	241	34.676	43.326	16.536	1.00 26.89
ATOM	1405	CB	ASP A		33.922	44.561	19.153	1.00 24.85
MOTA	1406	CG	ASP A		35.171	45.325	19.541	1.00 24.81
MOTA	1407	OD1	ASP A	241	35.144	46.032	20.567	1.00 27.86
MOTA	1408	OD2	ASP A	241	36.180	45.226	18.817	1.00 25.69
		N	HIS A			45.517		
MOTA	1409				34.913		15.960	1.00 26.86
MOTA	1410	CA	HIS A		35.853	45.222	14.852	1.00 27.45
ATOM	1411	С	HIS A	242	37.197	44.613	15.221	1.00 25.41
ATOM	1412	0	HIS A		37.871	43.998	14.347	1.00 23.94
MOTA	1413	CB	HIS A		36.085	46.481	14.013	1.00 32.38
ATOM	1414	CG	HIS A	242	34.858	46.957	13.304	1.00 37.46
ATOM	1415		HIS A		33.822	47.591	13.956	1.00 39.65
ATOM	1416		HIS A		34.472	46.837	12.011	1.00 39.29
MOTA	1417	CE1	HIS A		32.850	47.840	13.096	1.00 40.56
MOTA	1418	NE2	HIS A	242	33.219	47.392	11.909	1.00 40.36
ATOM	1419	N	SER A		37.615		16.471	
					,			1.00 22.23
MOTA	1420	CA	SER A		38.915	44.184	16.877	1.00 22.06
ATOM	1421	C	SER A	243	38.843	42.667	17.011	1.00 20.51
MOTA	1422	0	SER A	243	39.897	41.986	17.130	1.00 23.23
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MOTA	1423	СВ	SER A	243	39.368	44.785	18.211	1.00 22.47
MOTA	1424	OG	SER A		38.515	44.386	19.274	1.00 23:32
ATOM	1425	N	LEU A		37.635	42.115	16.979	1.00 20.52
ATOM	1426	CA	LEU A		37.454	40.649	17.145	1.00 18.32
ATOM	1427	C	LEU A		37.535	39.844	15.860	1.00 18.66
ATOM	1428	0	LEU A		37.482	38.576	15.892	1.00 18.25
ATOM	1429	CB	LEU A		36.120	40.368	17.843	1.00 18.23
	1430	CG	LEU A		35.998	41.054	19.206	1.00 13.01
MOTA							19.885	
ATOM	1431		LEU A		34.689	40.666		1.00 17.04
ATOM	1432		LEU A		37.189	40.661	20.063	1.00 19.23
MOTA	1433	И	TYR A		37.666	40.522	14.729	1.00 18.73
MOTA	1434	CA	TYR A		37.756	39.795	13.459	1.00 19.72
MOTA	1435	С	TYR A		38.536	40.545	12.398	1.00 20.55
ATOM	1436	0	TYR A		38.819	41.771	12.542	1.00 21.10
MOTA	1437	CB	TYR A		36.357	39.494	12.924	1.00 19.56
MOTA	1438	CG	TYR A		35.606	40.708	12.421	1.00 20.40
MOTA	1439	CD1	TYR A	245	34.977	41.586	13.302	1.00 20.11
MOTA	1440	CD2	TYR A	245	35.512	40.966	11.055	1.00 20.70
MOTA	1441	CE1	TYR A	245	34.265	42.689	12.834	1.00 21.90
MOTA	1442	CE2	TYR A	245	34.809	42.060	10.573	1.00 22.10
MOTA	1443	CZ	TYR A	245	34.184	42.919	11.466	1.00 23.05
ATOM	1444	OH	TYR A	245	 3.3.476	43.993	10.979	1.00 22.53
MOTA	1445	N	THR A	246	38.902	39.829	11.340	1.00 20.48
MOTA	1446	CA	THR A	246	39.621	40.429	10.195	1.00 19.46
MOTA	1447	С	THR A	246	38.811	40.054	8.964	1.00 19.29
MOTA	1448	0	THR A	246	37.999	39.085	9.000	1.00 16.84
MOTA	1449	CB	THR A	246	41.049	39.865	10.031	1.00 19.69
MOTA	1450	OG1	THR A	246	40.997	38.434	9.953	1.00 20.05
MOTA	1451	CG2	THR A	246	41.929	40.294	11.194	1.00 19.01
MOTA	1452	N	GLY A		 38.996	40.793	7:879	1.00 19.48
ATOM .	1453	CA	GLY A		38.259	40.490	6.668	1.00 19.61
ATOM	1454	C	GLY A		36.812	40.927	6.747	1.00 20.26
ATOM	1455	Ö	GLY A		36.412	41.712	7.660	1.00 21.64
ATOM	1456	N	SER A		36.006	40.437	5.816	1.00 21.23
MOTA	1457	CA	SER A		34.580	40.806	5.765	1.00 23.54
MOTA	1458	C	SER A		33.649	39.836	6.484	1.00 23.00
ATOM	1459	.0	SER A		33.978	38.625	6.684	1.00 21.96
MOTA	1460	СВ	SER A		34.135	40.936	4.304	1.00 24.06
ATOM	1461	:OG	SER A		34.814	41.999	3.656	1.00 28.27
ATOM	1462	N	LEU A		32.494	40.355	6.881	1.00 23.33
ATOM	1463	CA	LEU .A		31.453	39.551	7.550	1.00 23.71
ATOM		·C	LEU A		30.478	39.103	6.468	1.00 23.26
		0	LEU A			39.958		1.00 24.66
ATOM	•		LEU A		30.687			
ATOM'	1467	CG	LEU A		31.234	40.585	9.992	1.00 23.68
MOTA	1468		LEU A		30.483	41.728	10.659	1.00 23.07
MOTA	1469		LEU A		31.077		10.802	1.00 22.16
MOTA	1470	N	TRP 7		30.285	37.797	6.335	
MOTA	1471	.CA	TRP 7		29.328	37.282	5.348	
MOTA			TRP		28.115	36.810	6.115	
ATOM	1473		TRP A		28.242	36.079	7 153	
ATOM	1474		TRP					1.00 19.15
	1475		TRP I			36.128	3 /11	1.00 19.10
ATOM					30.759	30.33/	3.4ET	1.00 19.10
ATOM			TRP /		32.061			
ATOM			TRP A		30.328	36.777		1.00 18.74
MOTA	1478		TRP A		32.470	37.418	2.214	
ATOM	.1479		TRP A		31.425	37.294	1.336	
MOTA			TRP A		29.118	36.554 37.594	1.386	
MOTA			TRP A					
ATOM			TRP A			36.853		
MOTA	1483		TRP A	-		37.369		1.00 17.98
ATOM	1484	. N	TYR .	A 251	26.939	37.203	5.544	1.00 17.22

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ATOM	1485	CA	TYR A	251	25.699	36.825	6.328	1.00 16.85
ATOM	1486	C	TYR A		24.875	35.751		
MOTA	1487.				_		5.642	1.00 16.82
			TYR A		24.668	35.782	4.397	1.00 17.05
MOTA	1488	CB	TYR A		24.814	38.059	6.536	1.00 17.46
ATOM	1489	CG	TYR A	. 251	25.389	39.070	7.493	1.00 17.27
MOTA	1490	CD1	TYR A	251	26.265	40.065	7.055	1.00 18.34
MOTA	1491	CD2	TYR A	251	25.076	39.018	8.852	1.00 16.39
ATOM	1492	CE1	TYR A		26.819	40.984	7.955	
ATOM	1493	CE2	TYR A		25.622			1.00 18.20
						39.925	9.753	1.00 17.81
MOTA	1494	CZ	TYR A		26.487	40.900	9.302	1.00 17.43
MOTA	1495	OH	TYR A		27.014	41.779	10.215	1.00 20.25
ATOM	1496	N	THR A	252	24.395	34.803	6.436	1.00 15.07
ATOM	1497	CA	THR A	252	23.525	33.725	5.933	1.00 14.48
MOTA	1498	.C	THR A	252	22.204	33.996	6.646	1.00 16.15
MOTA	1499	0	THR A	252	22.193	34.429	7.845	1.00 16.66
ATOM	1500	СВ	THR A		24.056	32.325		1.00 14.69
ATOM	1501	OG1	THR A		23.273	31.316	5.684	1.00 14.03
ATOM	1502	CG2	THR A			32.118		
					23.974		7.839	1.00 14.05
ATOM	1503	N	PRO A		21.070	33.774	5.972	1.00 15.93
ATOM	1504	CA	PRO A		19.826	34.054	6.694	1.00 17.09
ATOM	1505	С	PRO A		19.418	33.029	7.741	1.00 18.67
ATOM	1506	0	PRO A	253	19.782	31.813	7.653	1.00 17.11
MOTA	1507	CB	PRO A	253	18.789	34.161	5.572	1.00 17.20
ATOM	1508	CG	PRO A	253	19.304	33.207	4.545	1.00 17.18
ATOM	1509	CD	PRO A	253	20.809	33.468	4.553	1.00 17.14
ATOM	1510	N	ILE A		18.692	33.501	8.750	1.00 18.82
ATOM	1511	CA	ILE A		18.165			
ATOM	1512	C				32.604	9.792	1.00 20.14
			ILE A		16.885	32.091	9.137	1.00 21.33
MOTA	1513	0	ILE A		15.911	32.875	8.914	1.00 21.52
ATOM	1514	CB	ILE A		17.827	33.368	11.091	1.00 20.62
ATOM	1515	CG1	ILE A	254	19.124	33.752	11.806	1.00 20.82
MOTA	1516	CG2	ILE A	254	16.935	32.509	11.994	1.00 19.41
ATOM	1517	CD1	ILE A	254	18.920	34.458	13.127	1.00 22.19
ATOM	1518	N	ARG A	255	16.868	30.810	8.795	1.00 22.06
ATOM	1519	CA	ARG A		15.702	30.211	8.115	1.00 23.47
ATOM	1520	C	ARG A		14.398	30.343	8.880	1.00 24.68
ATOM	1521	0	ARG A		13.334	30.719	8.299	1.00 25.49
ATOM	1522	CB	ARG A		15.951			
						28.735	7.852	1.00 22.62
ATOM	1523	CG	ARG A		14.843	28.093	7.053	1.00 22.10
ATOM	1524	CD	ARG A		14.985	26.598	7.069	1.00 22.76
MOTA	1525	ΝE	ARG A		14.031	25.958	6.176	1.00 22.51
MOTA	1526	CZ	ARG A		13.692	24.679	6.256	1.00 22.37
MOTA	1527	NH1	ARG A	255	14.232	23.914	7.195	1.00 20.91
MOTA	1528	NH2	ARG A	255	12.819	24.166	5.396	1.00 23.78
ATOM	1529	N	ARG A	256	14.451	30.023	10.165	1.00 24.98
MOTA	1530	CA	ARG A	256	13.264	30.085	11.029	1.00 25.56
ATOM	1531	С	ARG A		13.723	30.441	12.438	1.00 24.84
ATOM	1532	Ō	ARG A		14.829	30.013	12.893	1.00 22.14
ATOM	1533	CB	ARG A					
					12.561	28.729	11.009	1.00 27.37
ATOM	1534	CG	ARG A		11.350	28.599	11.914	1.00 29.24
ATOM	1535	CD	ARG A		10.878	27.150	11.899	1.00 29.60
ATOM	1536	NE	ARG A		10.180	26.788	13.126	1.00 31.29
MOTA	1537	CZ	ARG A	256	10.043	25.543	13.563	1.00 31.25
MOTA	1538	NH1	ARG A	256	10.559	24.535	12.870	1.00 31.19
MOTA	1539		ARG A		9.398	25.307	14.698	1.00 32.97
MOTA	1540	N	GLU A		12.914	31.219	13.141	1.00 24.01
ATOM	1541	CA	GLU A		13.270	31.650	14.500	1.00 24.01
ATOM	1542	C	GLU A					
					12.829	30.739	15.636	1.00 23:02
MOTA	1543	0	GLU A		11.749	30.947	16.264	1.00 26.15
MOTA	1544	CB	GLU A		12.739	33.055	14.748	1.00 23.25
MOTA	1545	CG	GLU A		13.439	34.123	13.930	1.00 26.24
MOTA	1546	CD	GLU A	257	12.572	35.353	13.746	1.00 27.27

ATOM	1547	OE1	GLU	А	257	13.124	36.470	13.673	1.00 27.35
ATOM	1548		GLU			11.334	35.197	13.665	1.00 30.46
	1549	N			258.	13.632	29.719	15.898	1.00 19.64
ATOM			TRP			13.390	28.798		1.00 19.75
MOTA	1550	CA						17.016	
MOTA	1551	С			258	14.812	28.548	17.495	1.00 19.46
MOTA	1552	0	TRP	Ä	258	15.267	29.190	18.500	1.00 20.47
ATOM	1553	CB	TRP	Α	258	12.632	27.537	16.561	1.00 18.27
MOTA	1554	CG	TRP	Α	258	13.203	26.710	15.455	1.00 17.96
MOTA	1555	CD1	TRP	А	258	13.898	27.143	14.364	1.00 18.43
ATOM	1556		TRP			13.051	25.293	15.298	1.00 17.87
ATOM	1557		TRP			14.187	26.082	13.537	1.00 18.62
MOTA	1558		TRP			13.678	24.935	14.088	1.00 17.86
MOTA	1559.		TRP			12.441	24.291	16.067	1.00 17.50
			TRP			13.717	23.614	13.624	1.00 19.19
ATOM	1560						22.976		1.00 19.16
ATOM	1561		TRP			12.477		15.608	
MOTA	1562		TRP			13.113	22.650	14.396	1.00 18.86
MOTA	1563	N	TYR			15.538	27.670	16.814	1.00 18.33
MOTA	1564	CA			259	16.965	27.458	17.126	1.00 15.42
MOTA	1565	С			259	17.550	28.474	16.157	1.00 16.46
MOTA	1566	0			259	16.789	29.066	15.323	1.00 15.71
ATOM	1567	CB			259	17.439	26.078	16.671	1.00 13.86
MOTA	1568	CG			259	17.056	24.927	17.564	1.00 13,98
ATOM	1569	CD1	TYR	А	259	17.876	24.539	18.627	1.00 13.32
ATOM	1570	CD2	TYR	Α	259	15.875	24.224	17.346	1.00 12.14
ATOM	1571	CE1	TYR	Α	259	17.520	23.467	19.450	1.00 15.06
ATOM	1572	CE2	TYR	Α	259	15.510	23.167	18.155	1.00 14.24
MOTA	1573	CZ	TYR	Α	259	16.329	22.789	19.200	1.00 14.26
ATOM	1574	OH			259	15.940	21.719	19.955	1.00 12.92
ATOM	1575	N			260	18.851	28.725	16.224	1.00 14.50
MOTA	1576	CA			260	19.440	29.630	15.232	1.00 15.21
ATOM	1577	C			260	19.716	28.718	14.037	1.00 15.90
ATOM	1578	:0			260	20.866	28.210	13.836	1.00 16.76
ATOM	1579	СВ			260	20.722	30.269	15.759	1.00 13.84
ATOM	1580	CG			260	20.426	31.416	16.690	1.00 14.32
	1581	CD1			260	20.534	31.270	18.078	1.00 13.41
ATOM					260	19.996	32.642	16.187	1.00 13.45
ATOM	1582	CD2				20.224	32.320	18.933	1.00 13.45
ATOM	1583	CE1			260		33.699		1.00 13.13
MOTA	1584	CE2			260	19.680	•	17.037	
ATOM	1585	CZ			260	19.801	33.530	18.404	1.00 13.22
MOTA	1586	OH .			260	19.531	34.582	19.239	1.00 12.88
111011	1587	N			261	18.664	28.476	13.260	1.00 15.81
MOTA	1588	CA			261	18.741	27.586	12.081	1.00 17.54
MOTA	1589	С			261	19.191	28.266	10.791	1.00 17.31
MOTA	1590	0			261		29.355	10.402	1.00 16.63
ATOM	1591	CB			261		26.914	11.842	1.00 16.53
MOTA	1592	ÇG			261		26.076	10.573	1.00 19.47
MOTA	1593	CD	GLU	A	261	15.965		10.326	1.00 20.18
MOTA	1594	OE1	GLU	Α	261	14.956	26.037	10.766	1.00 21.27
MOTA	1595	OE2	GLU	. A	261	15.902	24.390	9.673	1.00 20.94
ATOM	1596	N	VAL	Α	262	20.153	27.640	10.122	1.00 16.45
MOTA	1597	CA	VAL	A	262	20.679	28.147	8.842	1.00 16.13
ATOM	1598	С	VAL	Α	262	20.620	27.006	7.831	1.00 17.33
MOTA	1599	Ö			262	20.168	25.863	8.166	1.00 17.30
ATOM	1600	СВ			262	22.131	28.624	8.982	1.00 14.58
ATOM	1601				262	22.218	29.690	10.064	1.00 14.84
ATOM	1602				262	23.039	27.449	9.308	1.00 14.53
ATOM	1603	N			263	21.064	27.271	6.608	1.00 17.34
ATOM	1604	CA			263	21.044	26.245	5.554	1.00 16.67
ATOM	1605	C			263		26.042	4.931	1.00 16.64
ATOM	. 1606	0			263	00 054	27.016	4.418	1.00 17.50
		_			. 263°,		26.619	4.445	1.00 18.45
ATOM	1607	CB				18.608	26.522	4.996	1.00 18.90
MOTA	1608	CGI	. Lli	Α.	. 263	10.000	20.324	4.220	2.20 20.20

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MOTA	1609	CG2	ILE A 26	3 20	.192 2	5.694	3.243	1.00	18.17
ATOM	1610	CD1	ILE A 26			6.974	4.023		23.31
MOTA	1611	N	ILE A 26			4.802	4.988		16.67
ATOM	1612	CA	ILE A 26			4.413	4.409		14.63
MOTA	1613	C	ILE A 26			3.836	3.031		
									16.44
ATOM	1614	0	ILE A 26			2.915	2.908		13.53
ATOM	1615	CB	ILE A 26			3.320	5.253		14.79
ATOM	1616	CG1	ILE A 26			3.855	6.657		12.53
MOTA	1617	CG2	ILE A 26			2.846	4.563	1.00	12.07
MOTA	1618	CD1	ILE A 26	4 25	.685 2	2.799	7.615	1.00	12.69
MOTA	1619	N	VAL A 26	5 24	.546 2	4.334	1.992	1.00	17.37
ATOM	1620	CA	VAL A 26	5 24	.258 2	3.841	0.627	1.00	18.64
ATOM	1621	С	VAL A 26	5 25	.368 2	3.004	0.006	1.00	19.95
ATOM	1622	0	VAL A 26	5 25	.202 2	2.455	-1.127	1.00	19.29
MOTA	1623	СВ	VAL A 26				-0.322		18.56
ATOM	1624	CG1				5.901	0.287		16.70
ATOM	1625	CG2	VAL A 26				-0.590		17.47
ATOM	1626	N	ARG A 26			2.872	0.707		20.42
ATOM	1627	CA	ARG A 26			2.098	0.165		20.48
ATOM	1628	C	ARG A 26			2.044	1.162		19.59
ATOM	1629	0	ARG A 26			3.055	1.885		19.51
ATOM	1630	CB	ARG A 26	·			-1.129		22.33
ATOM	1631	CG	ARG A 26				-1.713		22.40
ATOM	1632	CD	ARG A 26				-2.789		24.49
MOTA	1633	NE	ARG A 26				-3.322		24.49
MOTA	1634	CZ	ARG A 26				-4.528		26.46
MOTA	1635	NH1	ARG A 26				-5.349		25.31
MOTA	1636	NH2	ARG A 26				-4.920		27.88
MOTA	1637	N	VAL A 26			0.891	1.246		18.31
ATOM	1638	CA	VAL A 26			0.766	2.136		18.32
MOTA	1639	С	VAL A 26	7 31	.671 2	0.072	1.369		18.25
MOTA	1640	0	VAL A 26	7 31	.409 1	9.192	0.489	1.00	19.14
MOTA	1641	CB	VAL A 26	7 30	.248 1	9.974	3.456	1.00	18.72
MOTA	1642	CG1	VAL A 26	7 28	.784 1	9.645	3.547	1.00	18.30
MOTA	1643	CG2	VAL A 26	7 31	.112 1	8.728	3.554	1.00	17.65
MOTA	1644	N	GLU A 26	8 32	.903 2	0.471	1.647	1.00	16.18
ATOM	1645	CA	GLU A 26			9.848	0.990	1.00	17.71
ATOM	1646	С	GLU A 26	8 35	.169 1	9.546	1.970	1.00	16.08
MOTA	1647	0	GLU A 26			0.191	3.064		13.62
ATOM	1648	CB	GLU A 26			0.717	-0.177		18.50
ATOM	1649	CG	GLU A 26			2.207	0.030		22.46
ATOM	1650	CD	GLU A 26				-1.181	1.00	
MOTA	1651		GLU A 26			2.970	-2.237		20.91
ATOM	1652	OE2				3.703	-1.067		22.44
ATOM	1653	N	ILE A 26			8.531	1.623		13.57
ATOM	1654	CA	ILE A 26			8.112	2.418		13.89
ATOM	1655	C	ILE A 26			8.448	1.485		14.06
			ILE A 26			7.832			14.03
MOTA	.1656	0					0.386		
ATOM	1657	CB	ILE A 26			6.596	2.703		14.48
ATOM	1658	CG1	ILE A 26			6.239	3.327		14.59
ATOM	1659	CG2	ILE A 26			6.193	3.645		12.12
ATOM	1660	CD1				7.022	4.592		13.16
MOTA	1661	N	ASN A 27			9.431	1.872		14.16
ATOM	1662	CA	ASN A 27			.9.886	1.038		13.20
MOTA	1663	С	ASN A 27			0.177	-0.399		13.24
MOTA	1664	0	ASN A 27			9.714	-1.385		13.72
MOTA	1665	СВ	ASN A 27			.8.852	1.047		11.19
MOTA	1666	CG	ASN A 27			9.186	2.054		13.23
ATOM	1667	OD1	ASN A 27			0.224	2.790		13.62
MOTA	1668	ND2	ASN A 27	0 43	.454 1	.8.348	2.117	1.00	11.67
MOTA	1669	N	GLY A 27	1 38	.691 2	0.932	-0.540		13.07
MOTA	1670	CA	GLY A 27			1.302	-1.858	1.00	13.58

ATOM	1671	С	GT.Y	A 271		37.393	20.241	-2.564	1.00 14.87
ATOM	1672	Ö		A 271		36.704	20.545	-3.581	1.00 14.87
ATOM	1673	N		A 272		37.447	19.005	-2.076	
ATOM	1674	CA		A 272		36.674	17.914		1.00 14.64
ATOM	1675	C		A 272					1.00 14.45
ATOM					-	35.261	17.870	-2.140	1.00 15.83
	1676	0		A 272		35.050	17.717	-0.902	1.00 15.81
ATOM	1677	CB		A 272		37.357	16.561	-2.486	1.00 14.85
ATOM	1678	CG		A 272		36.692	15.421	-3.250	1.00 14.45
ATOM	1679	CD		A 272		37.499	14.135	-3.211	1.00 16.34
MOTA	1680			A 272		37.097	13.134	-2.535	1.00 20.05
MOTA	1681	NE2		A 272		38.633	14.121	-3.909	1.00 13.09
ATOM	1682	N		A 273		34.291	17.995	-3.035	1.00 16.17
MOTA	1683	CA		A 273		32.857	17.987	-2.686	1.00 17.89
ATOM	1684	C		A 273		32.388	16.612	-2.201	1.00 16.92
ATOM	1685	0		A 273		32.713	15.566	-2.831	1.00 16.53
ATOM	1686	CB		A 273		32.060	18.395	-3.930	1.00 20.38
ATOM	1687	CG		A 273		30.576	18.526	-3.665	1.00 20.89
ATOM	1688			A 273		29.827	18.788	-4.630	1.00 21.98
ATOM	1689	OD2		A 273		30.155	18.378	-2.503	1.00 22.40
MOTA	1690	N		A 274		31.639	16.576	-1.101	1.00 17.95
ATOM	1691	CA		A 274		31.117	15.285	-0.587	1.00 19.37
ATOM	1692	С	LEU .	A 274		30.092	14.805	-1.598	1.00 21.18
MOTA	1693	0	LEU .	A 274		29.702	13.603	-1.623	1.00 20.08
ATOM	1694	CB		A 274		30.451	15.455	0.783	1.00 18.46
MOTA	1695	CG		A 274		31.356	15.595	2.011	1.00 19.89
MOTA	1696			A 274		30.489	15.558	3.267	1.00 17.23
ATOM	1697	CD2		A 274		32.392	14.463	2.050	1.00 17.76
MOTA	1698	N		A 275		29.646	15.736	-2.431	1.00 24.29
MOTA	1699	CA	LYS	A 275		28.676	15.452	-3.501	1.00 29.08
ATOM	1700	С		A 275		27.439	14.715	-3.000	1.00 28.92
MOTA	1701	0		A 275		27.119	13.586	-3.464	1.00 30.50
ATOM	1702	CB		A 275		29.360	14.642	-4.608	1.00 30.50
MOTA	1703	CG	LYS .	A 275		28.720	14.818	-5.970	1.00 33.82
MOTA	1704	CD		A 275		29.476	14.059	-7.042	1.00 36.63
MOTA	1705	CE.		A 275		28.848	14.297	-8.408	1.00 38.29
MOTA	1706	NZ		A 275		28.742	15.759	-8.702	1.00 39.43
MOTA	1707	N		A 276		26.734	15.329	-2.063	1.00 30.55
MOTA	1708	CA		A 276		25.519	14.722	-1.505	1.00 30.03
MOTA	1709	С		A 276		24.319	15.592	-1.815	1.00 30.11
ATOM	1710	0		A 276		24.465	16.818	-2.117	1.00 28.94
MOTA	1711	CB		A 276		25.641	14.576	0.011	1.00 30.29
MOTA	1712	CG		A 276		26.706	13.605	0.469	1.00 30.69
ATOM	1713	SD		A 276		26.687	13.418	2.261	1.00 32.94
MOTA	1714	CE		A 276		25.174	12.457	2.477	1.00 31.04
ATOM	1715	N		A 277		23.136	14.994	-1.756	1.00 31.37
ATOM	1716	CA		A 277		21.906	15.750	-1.994	1.00 33.34
ATOM	1717	С		A 277		21.903	16.864	-0.955	1.00 33.96
MOTA	1718	0		A 277		22.070	16.608	0.278	1.00 30.80
ATOM	1719	СВ		A 27,7		20.682	14.85 1	-1.818	1.00 36.24
ATOM	1720	CG		A 277		19.377	15.595	-2.029	1.00 38.93
ATOM	1721			A 277		18.332	14.925	-2.168	1.00 42.69
ATOM	1,722	-		A 277		19.386	16.844	-2.049	1.00 39.38
ATOM	1723	N		A 278		21.732	18.089	-1.432	1.00.34.50
ATOM	1724	CA		A 278		21.725	19.294	-0.581	1.00 37.44
ATOM	1725	C		A 278		20.988	19.126	0.749	1.00 35.96
ATOM	1726	0		A 278		21.503	19.540	1.834	1.00 34.38
MOTA	1727	CB		A 278		21.108	20.460	-1.362	1.00 39.86
ATOM	1728	ŚG		A 278		21.760	22.075	-0.852	1.00 50.09
ATOM	1729	N		A 279		19.802	18.529	0.705	1.00 33.76
ATOM	1730	CA		A 279		19.003	18.359	1.931	
ATOM	1731	С		A 279		19.584	17.430	2.996	1.00 30.06
MOTA	1732	O _i	LYS	A 279		19.173	17.501	4.189	1.00 27.89

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MOTA	1733	CB	LYS A	279	17.574	17.939	1.567	1.00 34.74
MOTA	1734	CG	LYS A		17.459	16.765	0.612	1.00 39.08
MOTA	1735	CD	LYS A		17.576	15.429	1.326	1.00 41.32
ATOM	1736	CE	LYS A	279	17.185	14.289	0.393	1.00 42.86
ATOM	1737	NZ	LYS A	279	17.118	12.978	1.099	1.00 45.07
MOTA	1738	N	GLU A		20.525	16.570	2.621	1.00 27.06
ATOM	1739	CA	GLU A		21.141	15.659	3.612	1.00 26.22
ATOM	1740	С	GLU A	280	21.900	16.458	4.673	1.00 25.34
ATOM	1741	0	GLU A	280	21.920	16.074	5.886	1.00 23.01
ATOM	1742	CB	GLU A		22.109	14.693	2.928	1.00 27.98
	1743	CG	GLU A		21.459	13.725	1.946	1.00 31.24
MOTA								
MOTA	1744	CD	GLU A		20.486	12.765	2.610	1.00 32.55
ATOM	1745	OE1	GLU A	280	20.447	12.704	3.857	1.00 33.21
MOTA	1746	OE2	GLU A	280	19.763	12.058	1.878	1.00 34.72
ATOM	1747	N	TYR A	281	22.515	17.562	4.255	1.00 23.32
	1748	CA	TYR A		23.295	18.420	5.176	1.00 22.69
MOTA								
ATOM	1749	C	TYR A		22.415	19.082	6.219	1.00 23.40
\mathtt{ATOM}	1750	0	TYR A	281	22.904	19.470	7.327	1.00 23.11
MOTA	1751	CB	TYR A	281	24.035	19.515	4.400	1.00 20.26
MOTA	1752	CG	TYR A	281	24.958	18.993	3.328	1.00 19.39
ATOM	1753		TYR A		25.858	17.961	3.601	1.00 17.78
ATOM	1754	CD2			24.943	19.534	2.042	1.00 18.55
MOTA	1755	CE1			26.719	17.478	2.623	1.00 17.05
MOTA	1756	CE2	TYR A	281	25.808	19.058	1.051	1.00 18.53
ATOM	1757	CZ	TYR A	281	26.692	18.028	1.355	1.00 17.87
ATOM	1758	OH	TYR A		27.558	17.533	0.407	1.00 18.13
			ASN A		21.136	19.232	5.899	1.00 22.82
MOTA		, N						
MOTA	1760	CA	ASN A		20.194	19.881	6.820	1.00 23.17
MOTA	1761	С	ASN A	282	19.089	18.922	7.238	1.00 23.84
ATOM	1762	0	ASN A	282	17.987	19.366	7.685	1.00 21.83
ATOM	1763	CB	ASN A	282	19.598	21.111	6.137	1.00 22.42
ATOM	1764	CG	ASN A		20.665	22.018	5.549	1.00 23.90
MOTA	1765		ASN A		21.426	22.693	6.298	1.00 23.87
MOTA	1766	ND2			20.760	22.044	4.224	1.00 23.36
ATOM	1767	N	TYR A	283	19.343	17.623	7.102	1.00 25.74
MOTA	1768	CA	TYR A	283	18.322	16.633	7.472	1.00 28.01
MOTA	1769	С	TYR A		17.905	16.843	8.912	1.00 29.29
	1770	Õ	TYR A		18.686	16.572	9.881	1.00 27.50
ATOM								
MOTA	1771	CB	TYR A		18.810	15.200	7.280	
MOTA	1772	CG	TYR A		17.783	14.200	7.756	1.00 31.64
ATOM	1773	CD1	TYR A	283	16.428	14.374	7.460	1.00 32.38
MOTA	1774	CD2	TYR A	283	18.153	13.098	8.523	1.00 33.44
ATOM	1775	CE1	TYR A	283	15.468	13.479	7.919	1.00 33.96
	1776	CE2			17.201	12.194	8.987	1.00 35.48
ATOM								1.00 35.35
MOTA	1777	CZ	TYR A		15.860	12.392	8.683	
MOTA	1778	OH	TYR A		14.918	11.504	9.149	1.00 36.54
ATOM	1779	N	ASP A	284	16.665	17.299	9.043	1.00 30.23
ATOM	1780	CA	ASP A	284	16.026	17.638	10.312	1.00 28.41
ATOM	1781	C	ASP A		16.273	19.129	10.409	1.00 27.12
			ASP A		15.309	19.953	10.305	1.00 25.19
ATOM	1782	0_						1.00 23.13
ATOM	1783	CB	ASP A		16.684	16.928	11.494	
MOTA	1784	CG	ASP A	. 284	16.035	17.283	12.813	1.00 33.49
ATOM	1785	OD1	ASP A	284	16.520	16.815	13.860	1.00 37.38
ATOM	1786		ASP A		15.035	18.031	12.802	1.00 35.95
		N	LYS A		17.542	19.499	10.563	1.00 22.62
ATOM	1787							
MOTA	1788	CA	LYS A		17.914	20.927	10.678	1.00 20.42
ATOM	1789	С	LYS A	. 285	19.420	21.145	10.812	1.00 19.89
ATOM	1790	0	LYS A	285	20.209	20.174	11.037	1.00 19.63
ATOM	1791	CB	LYS A		17.230	21.540	11.903	1.00 18.63
ATOM	1792	CG	LYS A		17.753	20.987	13.232	1.00 16.63
						21.538	14.421	1.00 14.93
ATOM	1793	CD	LYS A		16.966			
MOTA	1794	CE	LYS A	. ∠85	17.551	21.088	15.754	1.00 15.57

ATOM	1795	NZ	LYS	Δ	285	-	17.482	19.606	15.974	1.00 13.50
ATOM	1796	N			286		19.827	22.402	10.678	1.00 17.19
ATOM	1797	CA	SER				21.241	22.808	10.827	1.00 16.52
ATOM	1798	C	SER	-			21.228	24.034	11.727	1.00 15.74
ATOM	1799	Ō	SER				20.592	25.080	11.377	1.00 14.46
ATOM	1800	СВ	SER				21.862	23.179	9.475	1.00 14.40
ATOM	1801	OG	SER			,	22.064	22.036	8.671	1.00 16.60
ATOM	1802	N	ILE				21.900	23.946	12.870	1.00 13.25
ATOM	1803	CA	ILE				21.933	25.079	13.805	1.00 13.23
ATOM	1804	C	ILE				23.342	25.511	14.206	1.00 15.14
ATOM	1805	0	ILE				24.346	24.750	14.024	1.00 13.14
ATOM	1806	CB	ILE				21.145	24.757	15.102	1.00 13.55
ATOM	1807	CG1	ILE				21.898	23.717	15.929	1.00 13.53
ATOM	1808	CG2	ILE				19.758	24.214	14.754	1.00 12.32
MOTA	1809		ILE				21.274	23.455	17.283	1.00 12.10
ATOM	1810	N	VAL				23.431	26.728	14.732	1.00 14.78
ATOM	1811	CA	VAL				24.701	27.292	15.223	1.00 15.54
MOTA	1812	C	VAL				24.510	27.262	16.733	1.00 16.05
ATOM	1813	0.	VAL				23.571	27.930	17.278	1.00 15.61
ATOM	1814	CB	VAL				24.896	28.751	14.767	1.00 15.19
ATOM	1815		VAL				26.248	29.259	15.239	1.00 14.78
ATOM	1816		VAL				24.791	28.842	13.246	1.00 15.19
ATOM	1817	N	ASP				25.355	26.512	17.430	1.00 15.91
MOTA	1818	CA	ASP				25.194	26.373	18.891	1.00 14.81
ATOM	1819	C	ASP				26.467	26.444	19.724	1.00 15.27
ATOM	1820	ō	ASP				27.322	25.504	19.700	1.00 15.75
ATOM	1821	CB	ASP				24.467	25.060	19.168	1.00 12.65
ATOM	1822	CG	ASP				24.264	24.806	20.634	1.00 13.29
ATOM	1823		ASP			•	24.372	25.768	21.426	1.00 11.88
ATOM	1824		ASP				23.981	23.639	20.988	•
ATOM	1825	N	SER				26.604	27.529	20.479	1.00 15.19
ATOM	1826	CA	SER				27.782	27.730	21.346	1.00 14.55
MOTA	1827	C ·	SER				27.770	26.748	22.510	1.00 15.43
ATOM	1828	0	SER				28.823	26.539	23.186	1.00 13.77
ATOM	1829	CB	SER				27.795	29.165	21.888	1.00 15.33
MOTA	1830	OG	SER				26.614	29.442	22.620	1.00 12.79
MOTA	1831	N	GLÝ	Α	291		26.612	26.137	22.759	1.00 14.34
MOTA	1832	CA	GLY	Α	291		26.486	25.192	23.856	1.00 14.93
ATOM	1833	С	GLY	Α	291		26.779	23.751	23.479	1.00 16.64
MOTA	1834	0	GLY	Α	291		26.502	22.792	24.277	1.00 14.49
MOTA	1835	N	THR	Α	292		27.305	23.556	22.277	1.00 16.47
ATOM	1836	CA	TĤR	A	292		27.674	22.202	21.812	1.00 15.30
MOTA	1837	С	THR			-	29.159		21.482	1.00 14.67
MOTA	1838	0 .			292	•	29.653	23.102	20.725	1.00 13.26
MOTA	1839	CB			292			21.784	20.550	1.00 15.29
MOTA	1840		THR				25,522	21.521	20.895	1.00 13.88
ATOM	1841		THR				27.514	20.527	19.932	1.00 13.59
MOTA	1842	N			293	-	29.887	21.253	22.027	1.00 14.43
MOTA	1843	CA			293		31.343	21.162	21.801	1.00 12.76
MOTA	1844	C			293	-	31.749	20.906	20.348	1.00 14.47
MOTA	1845	0			293		32.478	21.735.		1.00 14.61
ATOM	1846		THR				31.949	20.035	22.650	1.00 12.36
MOTA	1847		THR				31.726	20.304	24.041	1.00 10.79
MOTA	1848		THR				33.437	19.916	22.382	1.00 9.56
ATOM	1849	N			294		31.286	19.783		1.00 13.53
MOTA .	1.850	CA			294		31.648	19.349	18:440	1.00 15.26
ATOM	1851	·C			294		30.871	19.917		1.00 15.45
ATOM	1852	0			294		29.851	20.662	17.431	1.00 13.68
ATOM	1853	·CB			294		31.494	17.832	18.307	1.00 14.81
MOTA	1854	CG			294		32.351	17.051	19.270	1.00 14.13
ATOM	1,855		ASN				32.264	15.791		1.00 19.85
MOTA	1856	ND2	AŚŃ	A	294		33.174	17.734	20.051	1.00 13.25

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ATOM	1857	N	LEU A	295	31.365	19.556	16.096	1.00 15.21
MOTA	1858	CA	LEU A		30.689			
ATOM	1859		LEU A			19.866	14.835	1.00 15.29
		_			29.924	18.548	14.719	1.00 16.43
ATOM	1860	0	LEU A		30.556	17.452	14.575	1.00 16.34
ATOM	1861	CB	LEU A		31.674	19.963	13.671	1.00 13.54
MOTA	1862	CG	LEU A	295	31.017	19.837	12.287	1.00 14.74
MOTA	1863	CDI	L LEU A	295	29.991	20.947	12.109	1.00 14.37
MOTA	1864	CD2	LEU A	295	32.073	19.903	11.179	1.00 13.91
ATOM	1865	N	ARG A		28.606	18.591	14.831	1.00 15.91
ATOM	1866	CA	ARG A		27.827			
ATOM	1867	C	ARG A			17.349	14.719	1.00 17.47
					27.180	17.300	13.343	1.00 17.04
ATOM	1868	0	ARG A		26.655	18.339	12.840	1.00 15.28
ATOM.	1869		ARG A		26.785	17.290	15.834	1.00 18.37
MOTA	1870	CG	ARG A		27.421	17.444	17.208	1.00 19.73
ATOM	1871	CĐ	ARG A	296	26.425	17.262	18.324	1.00 22.63
MOTA	1872	NE	ARG A	296	26.292	15.867	18,722	1.00 25.23
ATOM	1873	CZ	ARG A	296	25.135	15.223	18.776	1.00 26.52
ATOM	1874	NH1			24.011	15.851	18.446	1.00 27.11
ATOM	1875	NH2			25.100	13.961	19.179	1.00 27.11
ATOM	1876	N	LEU A		27.211	16.123		
ATOM	1877	CA	LEU A		26.660		12.722	1.00 15.65
ATOM	1878		LEU A			15.945	11.356	1.00 15.33
ATOM		C			25.657	14.800	11.246	1.00 17.46
	1879	0	LEU A		25.795	13.743	11.938	1.00 16.37
ATOM	1880	СВ	LEU A		27.806	15.681	10.371	1.00 12.00
MOTA	1881	CG	LEU A		28.925	16.729	10.277	1.00 11.84
MOTA	1882	CD1		297	30.136	16.148	9.561	1.00 8.16
MOTA	1883	CD2	LEU A	297	28.410	17.962	9.559	1.00 8.99
ATOM	1884	N	PRO A	298	24.636	14.960	10.386	1.00 19.11
ATOM	1885	CA	PRO A	298	23.636	13.901	10.217	1.00 20.53
ATOM	1886	С	PRO A		24.387	12.619	9.868	1.00 21.03
MOTA	1887	Ō	PRO A		25.419	12.668	9.131	
ATOM	1888	СВ	PRO A					1.00 21.77
ATOM	1889	CG	PRO A		22.788	14.411	9.054	1.00 19.18
					22.861	15.897	9.209	1.00 20.46
ATOM	1890	CD	PRO A		24.335	16.111	9.517	1.00 19.69
ATOM	1891	N	LYS A		23.911	11.487	10.376	1.00 22.77
ATOM	1892	CA	LYS A		24.562	10.169	10.137	1.00 25.34
ATOM	1893	C	LYS A		25.169	9.979	8.753	1.00 24.56
ATOM	1894	0	LYS A		26.393	9.681	8.617	1.00 22.24
ATOM	1895	CB	LYS A	299	23.566	9.034	10.387	1.00 29.05
MOTA	1896	CG	LYS A	299	24.156	7.650	10.146	1.00 33.27
ATOM	1897	CD	LYS A	299	23.144	6.547	10.408	1.00 37.10
MOTA	1898	CE	LYS A	299	23.758	5.178	10.151	1.00 38.78
MOTA	1899	NZ	LYS A		22.775	4.077	10.380	1.00 42.51
ATOM	1900	N	LYS A		24.340	10.127	7.729	1.00 24.24
ATOM	1901	CA	LYS A		24.774	9.955	6.333	
ATOM	1902	C	LYS A					1.00 25.41
ATOM	1903	Ö	LYS A		25.901	10.916	5.952	1.00 24.12
					26.889	10.515	5.262	1.00 23.67
ATOM	1904	CB	LYS A		23.576	10.154	5.403	1.00 28.77
ATOM	1905	CG	LYS A		23.788	9.660	3.990	1.00 33.37
MOTA	1906	CD	LYS A		22.661	8.718	3.569	1.00 38.01
MOTA	1907	CE	LYS A		21.298	9.393	3.652	1.00 40.18
MOTA	1908	NZ	LYS A	300	20.191	8.455	3.291	1.00 42.69
ATOM	1909	N	VAL A	301	25.784	12.172	6.368	1.00 20.46
MOTA	1910	CA	VAL A	301	26.832	13.169	6.058	1.00 18.21
ATOM	1911	С	VAL A		28.083	12.842	6.867	1.00 17.93
ATOM	1912	Ō	VAL A		29.241	12.929	6.343	1.00 16.84
ATOM	1913	СВ	VAL A		26.358	14.601	6.391	
ATOM	1914		VAL A					1.00 17.29
ATOM	1914		VAL A		27.468	15.605	6.105	1.00 15.43
					25.118	14.935	5.565	1.00 16.34
ATOM	1916	N	PHE A		27.887	12.448	8.122	1.00 17.43
ATOM	1917	CA	PHE A		29.032	12.099	8.990	1.00 18.16
MOTA	1918	С	PHE A	302	29.854	10.957	8.399	1.00 18.95

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MOTA	1919	0	PHE A 302		31.121	11.004	8.399	1.00 18.60
MOTA	1920	CB	PHE A 302		28.550	11.713	10.391	1.00 17.38
ATOM	1921 -		PHE A 302		29.639	11.180	11.265	1.00 19.16
MOTA	1922	CD1	PHE A 302		29.866	9.810	11.362	1.00 17.81
MOTA	1923	CD2	PHE A 302		30.498	12.051	11.923	1.00 18.89
ATOM	1924	CE1	PHE A 302		30.934	.9.320	12.096	1.00 19.63
ATOM	1925	CE2	PHE A 302		31.573	11.569	12.660	1.00 19.90
MOTA	1926	CZ	PHE A 302		31.793	10.201	12.747	1.00 19.13
MOTA	1927	N	GLU A 303		29.172	9.931	7.901	1.00 19.20
ATOM	1928	CA	GLU A 303		29.859	8.769	7.295	1.00 21.56
ATOM	1929	С	GLU A 303		30.679	9.189	6.083	1.00 19.19
MOTA	1930	0	GLU A 303		31.865	8.777	5.929	1.00 18.04
ATOM	1931	CB	GLU A 303		28.836	7.704	6.888	1.00 24.72
ATOM	1932	CG	GLU A 303		28.246	6.939	8.069	1.00 29.90
MOTA	1933	CD	GLU A 303		27.051	6.076	7.683	1.00 33.77
ATOM	1934	OE1	GLU A 303		26.585	5.294	8.541	1.00 36.31
MOTA	1935	OE2			26.572	6.183	6.528	1.00 36.51
ATOM	1936	N	ALA A 304		30.088	9.998	5.216	1.00 17.86
MOTA	1937	CA	.ALA A 304		30.805	10.472	4.007	1.00 18.11 1.00 17.49
ATOM	1938	C	ALA A 304		31.999	11.354	4.386	1.00 17.49
ATOM	1939	0	ALA A 304		33.102	11.242	3.777 3.102	1.00 17.78
ATOM	.1940	CB	ALA A 304		29.849 31.812	11.244 12.221	5.377	1.00 17.14
ATOM	1941 1942	N	ALA A 305 ALA A 305		32.900	13.128	5.829	1.00 16.43
ATOM	1942	CA C	ALA A 305		34.092	12.387	6.440	1.00 16.39
ATOM ATOM	1943	0	ALA A 305		35.272	12.644	6.054	1.00 17.78
MOTA	1945		ALA A 305		32.351	14.140	6.833	1.00 15.92
ATOM	1946	N	VAL A 306		33.842	11.476	7.375	1.00 15.50
ATOM	1947	CA	VAL A 306		34.971	10.756	8.004	1.00 17.31
ATOM	1948	C	VAL A 306	•	35.719	9.920	6.987	1.00 16.95
ATOM	1949	Ō	VAL A 306		36.983	9.829	7.029	1.00 16.21
ATOM	1950	СВ	VAL A 306		34.514	9.845	9.162	1.00 17.93
ATOM	1951	CG1	VAL A 306		33.954	10.693	10.280	1.00 19.37
ATOM	1952	CG2			33.477	8.851	8.669	1.00 19.63
MOTA	1953	N	LYS A 307		34.987	9.307	6.065	1.00 17.11
ATOM .	1954	CA	LYS A 307		35.641	8.488	5.032	1.00 18.39 1.00 17.59
MOTA	1955	C	LYS A 307		36.654	9.350 8.959	4.279	1.00 17.39
MOTA	1956	0	LYS A 307		37.848 34.602	7.940	4.052	1.00 18.03
ATOM ATOM	1957 1958	CB CG	LYS A 307 LYS A 307		35.212	7.112	2.930	1.00 24.02
ATOM	1959	CD	LYS A 307		34.147	6.415	2.102	1.00 26.72
ATOM	1960	CE	LYS A 307		34.779	5.505	1.058	1.00 29.36
MOTA	1961	NZ	LYS A 307		33.745	4.869	0.193	1.00 31.68
ATOM	1962	N	SER A 308		36.205	10.520	3.842	
MOTA	:1963	CA	SER A 308		37.059	11.460	3.091	1.00 17.46
MOTA	1964	С	SER A 308		38.198	12.000	3.953	1.00 16.11
ATOM	1965	Ο	SER A 308		39.378	12.056	3.501	1.00 17.12
MOTA	1966	CB	SER A 3.08		36.208	12.620	2.560	1.00 17.51
ATOM	1967	.OG	SER A 3.08		36.982	13.505	1.774	1.00 19.76
MOTA	1968		.ILE A 309	•	37.886	12.400	5.180	1.00 16.07
MOTA	1969		ILE A 309		38.926	12.927	6.083	1.00 14.41 1.00 14.93
MOTA	1970	C	.ILE A 309		39.945	11.831	6.378	1.00 14.90
MOTA	1971		ILE A 309		41.171	12.112	6.505 7.401	1.00 13.88
MOTA	1972		ILE A 309		38.310 37.346	13.439 14.595		1.00 13.88
MOTA	1973		L'ILE A 309 2.ILE A 309	•	37.346			1.00 11.40
MOTA	1974 1975		1:ILE A 309		36.575			1.00 12.70
ATOM	1975		LYS A 310		39.475		6.485	•
ATOM ATOM	1977		LYS A 310		40.375			1.00 17.74
ATOM	1978		LYS A 310	•	41.289		5.559	
ATOM	1979		LYS A 310		42.532		5.715	1.00 16.87
ATOM			LYS A 310		39.577			1.00 18.35

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ATOM	1981	CG	LYS A	310	39.003	7.953	8.373	1.00 20.85
ATOM	1982	CD	LYS A	310	38.269	6.617	8.432	1.00 22.02
MOTA	1983	CE	LYS A		37.584	6.404	9.757	1.00 25.26
MOTA	1984	NZ	LYS A	310	36.808	5.129	9.752	1.00 26.15
ATOM	1985	N	ALA A	311	40.698	9.211	4.370	1.00 15.56
ATOM	1986	CA	ALA A		41.466	9.007	3.124	1.00 17.77
MOTA	1987	С	ALA A		42.549	10.071	2.990	1.00 17.36
ATOM	1988	0	ALA A	311	43.708	9.768	2.578	1.00 20.71
ATOM	1989	CB	ALA A	311	40.524	9.047	1.908	1.00 14.11
MOTA	1990	И	ALA A	312	42.210	11.309	3.330	1.00 16.63
ATOM	1991	CA	ALA A		43.184	12.418		
							3.235	1.00 15.73
MOTA	1992	C	ALA A		44.247	12.342	4.333	1.00 15.59
MOTA	1993	0	ALA A	312	45.348	12.958	4.207	1.00 13.09
ATOM	1994	CB	ALA A	312	42.449	13.758	3.301	1.00 13.50
ATOM	1995	N	SER A		43.950	11.593	5.393	1.00 17.05
MOTA	1996	CA	SER A		44.867	11.432	6.560	1.00 19.05
MOTA	1997	С	SER A		45.579	10.085	6.593	1.00 19.49
ATOM	1998	0	SER A	313	46.332	9.787	7.568	1.00 21.95
MOTA	1999	CB	SER A	313	44.075	11.555	7.865	1.00 17.23
ATOM	2000	OG	SER A	313	43.501	12.834	8.003	1.00 23.58
ATOM	2001	N	SER A		45.368	9.270	5.570	1.00 20.76
	.2002	CA	SER A		45.952	7.909	5.513	1.00 22.73
MOTA	2003	C	SER A	314	47.436	7.725	5.838	1.00 21.90
ATOM	2004	0	SER A	314	47.825	6.639	6.359	1.00 20.76
MOTA	2005	CB	SER A	314	45.650	7.271	4.150	1.00 22.50
ATOM	2006	OG	SER A		46.207	8.032	3.093	1.00 27.94
MOTA	2007	N	THR A		48.285	8.714	5.570	1.00 20.90
MOTA	2008	CA	THR A		49.732	8.523	5.868	1.00 23.78
MOTA	2009	С	THR A	315	50.020	8.454	7.361	1.00 25.42
ATOM	2010	0	THR A	315	51.191	8.219	7.784	1.00 26.24
ATOM	2011	CB	THR A	315	50.616	9.634	5.257	1.00 23.59
ATOM	2012	OG1	THR A		50.256	10.901	5.818	1.00 22.73
	2013	CG2	THR A		50.456	9.668	3.745	1.00 22.79
ATOM								
MOTA	2014	N	GLU A		48.994	8.655	8.176	1.00 27.46
MOTA	2015	CA	GLU A	316	49.170	8.589	9.638	1.00 29.81
MOTA	2016	C	GLU A	316	48.258	7.503	10.201	1.00 30.55
ATOM	2017	0	GLU A	316	47.110	7.314	9.710	1.00 29.51
ATOM	2018	СB	GLU A		48.819	9.931	10.279	1.00 32.51
ATOM	2019	CG	GLU A		49.277	10.039	11.725	1.00 36.72
MOTA	2020	CD	GLU A		50.571	10.818	11.879	1.00 36.99
ATOM	2021	OE1	GLU A	316	51.456	10.728	11.003	1.00 37.39
ATOM	2022	OE2	GLU A	316	50.704	11.522	12.893	1.00 41.14
MOTA	2023	N	LYS A	317	48.736	6.775	11.205	1.00 32.69
ATOM	2024	CA	LYS A		47.928	5.702	11.828	1.00 35.09
ATOM	2025	C	LYS A		47.216	6.223	13.071	1.00 33.44
MOTA	2026	0	LYS A		47.804	7.005	13.883	1.00 34.13
ATOM	2027	CB	LYS A	317	48.809	4.505	12.202	1.00 38.52
MOTA	2028	CG	LYS A	317	49.980	4.844	13.106	1.00 43.41
ATOM	2029	CD	LYS A	317	50.665	3.588	13.638	1.00 46.99
ATOM	2030	CE	LYS A		51.165	2.686	12.514	1.00 48.65
	2031							1.00 49.49
ATOM		NZ	LYS A		51.731	1.410	13.043	
ATOM	2032	N	PHE A		45.965	5.818	13.245	1.00 31.00
ATOM	2033	CA	PHE A	318	45.188	6.272	14.408	1.00 30.33
ATOM	2034	С	PHE A	318	44.683	5.120	15.263	1.00 30.57
ATOM	2035	Ō	PHE A		44.171	4.088	14.732	1.00 29.80
ATOM	2036	CB	PHE A		44.014	7.135	13.944	1.00 28.83
ATOM	2037	CG	PHE A		44.436	8.367	13.197	1.00 28.31
MOTA	2038		PHE A		44.625	8.333	11.817	1.00 27.09
ATOM	2039	CD2	PHE A	318	44.686	9.554	13.879	1.00 27.59
ATOM	2040	CE1	PHE A	318	45.060	9.466	11.130	1.00 27.37
ATOM	2041	CE2	PHE A	318	45.122	10.691	13.200	1.00 26.98
MOTA	2042	CZ	PHE A		45.309	10.648	11.826	1.00 27.12
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MOTA	2043	N	DDO	A 319		44.805	5.252	16.591	1.00 30.02
			_						
ATOM	2044	CA	PRO	A 319		44.361	4.222	17.535	1.00 30.20
ATOM	2045.	С	PRO	A 319		42.864	3.977	17.460	1.00 29.88
MOTA	2046	0	ЬКÓ	A 319		42.087	4.882	17.040	1.00 29.27
ATOM	2047	CB	PRO	A 319		44.777	4.793	18.890	1.00 30.49
ATOM	2048	CG		A 319					
						44.667	6.276	18.674	1.00 31.99
ATOM .	2049	CD	PRO	A 319		45.308	6.437	17.309	1.00 30.77
ATOM	2050	N		A 320		42.449	2.779	17.860	1.00 30.08
MOTA	2051	CA	ASP	A 320		41.018	2.389	17.867	1.00 29.79
ATOM	2052	С	ASP	A 320		40.183	3.406	18.652	1.00.28.71
ATOM		Ō							
	2053			A 320		40.560	3.804	19.804	1.00 27.90
ATOM	2054	CB	ASP	A 320		40.855	1.009	18.520	1.00 31.81
ATOM	2055	CG	ACD	A 320		41.545	-0.104	17.740	1.00 34.27
MOTA	2056			A 320		41.787	-1.182	18.331	1.00 34.13
MOTA	2057	OD2	ASP	A 320		41.833	0.092	16.538	1.00 35.41
ATOM	2058	N		A 321		39.067	3.837	18.068	1.00 26.34
MOTA	2059	CA	GLY	A 321		38.193	4.781	18.745	1.00 24.91
MOTA	2060	С	GLY	A 321		38.439	6.259	18.490	1.00 23.96
ATOM	2061	Ō		À 321		37.632	7.129	18.941	1.00 23.66
MOTA	2062	N,	PHE	A 322		39.519	6.591	17.793	1.00 22.07
ATOM	2063	CA	PHE	A 322		39.810	8.011	17.507	1.00 20.41
MOTA	2064	C,		A 322		38.705	8.670	16.684	1.00 20.53
MOTA	2065	0	PHE	A 322		38.157	9.743	17.078	1.00 20.75
ATOM	2066	CB	PHE	A 322		41.126	8.157	16.747	1.00 19.07
ATOM	2067	CG		A 322			9.567		1.00 19.05
						41.405		16.306	
MOTA	2068	CD1	PHE	A 322		41.701	10.555	17.240	1.00 17.04
MOTA	2069	CD2	PHE	A 322		41.326	9.918	14.960	1.00 17.20
MOTA	2070			A 322		41.912	11.872	16.840	1.00 18.99
MOTA	2071 ⁻	CE2	PHE	A 322		41.535	11.229	14.552	1.00 17.99
ATOM	2072	CZ	PHE	A 322		41.829	12.210	15.494	1.00 16.28
ATOM	2073	N		A 323		38.367	8.063	15.552	1.00 20.75
	. 2074	CA		A 323		37.330	8.622	14.664	1.00 22.37
ATOM	2075	С	TRP	A 323	•	35.940	8.626	15.273	1.00 23.50
MOTA	2076	Ο.	TRP	A 323		35.036	9.379	14.804	1.00 22.84
MOTA	2077	СВ		A 323		37.322	7.872	13.335	1.00 21.45
ATOM	2078	CG	TRP	A. 323		38.643	7.924	12.664	1.00 20.71
ATOM .	2079	CD1		A 323		39.566	6.921	12.594	1.00 20.50
ATOM	2080	CD2		A 323		39.217	9.049	11.986	1.00 20.31
ATOM	2081	NE1	TRP	A 323		40.679	7.349	11.913	1.00 20.18
MOTA '	2082	CE2	TRP	A 323		40.492	8.651		1.00 20.95
MOTA	2083	CE3		A 323		38.778	10.354		1.00 20.80
ATOM	2084	CZ2	\mathtt{TRP}	A 323		41.337	9.511	10.816	1.00 20.49
ATOM	2085	C23		A 323		39.618	11.212	11.013	1.00 21.58
ATOM	2086								1.00 21.15
				A 323		40.885	10.784	10.569	
ATOM	2087	N	LEU	A 324		35.734	7.810	16.300	1.00 26.13
ATOM	2088	CA	LEU	A 324		34.428	7.772	16.983	1.00 27.96
ATOM	2089	C							
				A 324		34.417	8.877	18.040	1.00 29.09
MOTA	2090	0	LEU	A 324		33.413	9.044	18.799	1.00.29.23
MOTA	2091	СВ	LEU	A 324		34.202	6.408	17.642	1.00 29.11
MOTA	2092	CG		A 324					1.00 30.04
						33.910	5.236	16.697	
MOTA	2093	CD1	LEU	A 324		33.791	3.948	17.501	1.00 30.31
MOTA	2094			A 324		32.625	5.499	15.924	1.00 29.47
ATOM	2095	Ņ							
,				A 325		35.513	9.634	18.098	1.00 29.34
MOTA	2096	CA		A 325	•	35.632	10.728	19.048	1.00 30.68
MOTA	2097	С	GLY	A 325		35.794	10.280	20.489	1.00: 31.19
ATOM	2098			A 325					1.00 31.53
						35.687	11.109	21.442	
ATOM'	2099	N	GLU	A 326	•	36.067	8.995	20.683	1.00 32.22
ATOM	2100	CA	GLU:	A 326	٠.	36.225	8.436	22.042	1.00 34.09
MOTA	2101	Ċ	-	A 326				22.563	1.00.33.56
						37.655	8.482		
MOTA	2102	0		A 326		37 [.] .907	8.933	23.720	1.00 34.19
ATOM .	2103	CB	GLU	A 326		35.728	6.992	22.062	1.00 35.56
	2104	CG		A 326	•	34.267	6.847.		1.00 38.03
				520		33.207	0.04/	22.003	

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\mathtt{ATOM}	2105	CD	GLU A	326	33.855	5.401	21.494	1.00 40.36
ATOM	2106	OE1	GLU A	326	32.662	5.162	21.207	1.00 41.84
ATOM	2107.	OE2	GLU A		34.720	4.506	21.626	
								1.00 42.10
ATOM	2108	N	GLN A		38.602	8.031	21.750	1.00 32.81
ATOM	2109	CA	GLN A	327	40.009	8.017	22.178	1.00 31.36
MOTA	2110	С	GLN A	327	40.844	9.142	21.608	1.00 30.14
ATOM	2111	0	GLN A	327	40.612	9.626	20.458	1.00 28.97
ATOM	2112	CB	GLN A		40.650	6.667	21.842	1.00 34.41
ATOM	2113							
		CG	GLN A		40.770	5.749	23.060	1.00 38.96
MOTA	2114	CD	GLN A		39.443	5.546	23.778	1.00 40.61
MOTA	2115	OE1			39.410	5.223	25.002	1.00 42.73
ATOM	2116	NE2	GLN A	327	38.344	5.714	23.053	1.00 42.75
ATOM	2117	N	LEU A	328	41.814	9.581	22.394	1.00 28.01
MOTA	2118	CA	LEU A	328	42.695	10.663	21.964	1.00 28.64
ATOM	2119	С	LEU A		43.889	10.100	21.219	1.00 27.50
ATOM	2120	Ō	LEU A		44.207	8.873	21.317	
	2121							
ATOM		CB	LEU A		43.177	11.467	23.180	1.00 29.39
ATOM	2122	CG	LEU A		43.924	10.735	24.304	1.00 31.09
MOTA	2123	CD1		_	45.298	10.283	23.831	1.00 31.75
MOTA	2124	CD2	LEU A	328	44.074	11.669	25.498	1.00 31.12
ATOM	2125	N	VAL A	329	44.539	10.961	20.449	1.00 25.26
ATOM	2126	CA	VAL A	329	45.748	10.583	19.722	1.00 23.64
MOTA	2127	C	VAL A		46.779	11.593	20.203	1.00 23.76
MOTA	2128	Ō	VAL A		46.431	12.786	20.476	1.00 21.96
ATOM	2129	CB						
			VAL A		45.560	10.675	18.194	1.00 23.82
MOTA	2130	CG1	VAL A		45.100	12.070	17.794	1.00 23.64
MOTA	2131	CG2	VAL A		46.866	10.317	17.501	1.00 23.70
MOTA	2132	N	CYS A	330	48.025	11.157	20.344	1.00 23.69
ATOM	2133	CA	CYS A	330	49.088	12.046	20.830	1.00 24.17
ATOM	2134	C	CYS A	330	50.315	12.060	19.937	1.00 23.87
MOTA	2135	0	CYS A		50.592	11.089	19.165	1.00 24.32
MOTA	2136	CB	CYS A		49.548	11.633	22.228	1.00 24.93
	2137							
MOTA		SG	CYS A		48.353	11.638	23.608	1.00 29.07
ATOM	2138	И	TRP A		51.069	13.144	20.047	1.00 22.66
ATOM	2139	CA	TRP A		52.306	13.318	19.281	1.00 22.40
ATOM	2140	С	TRP A	331	53.333	13.972	20.177	1.00 22.22
MOTA	2141	0	TRP A	331	52.979	14.698	21.154	1.00 21.57
ATOM	2142	CB	TRP A	331	52.069	14.207	18.064	1.00 21.16
ATOM	2143	CG	TRP A	331	51.345	13.524	16.959	1.00 19.61
ATOM	2144	CD1	TRP A		51.868	12.634	16.067	1.00 18.33
ATOM	2145	CD2	TRP A		49.966	13.684		
						•	16.606	1.00 18.42
ATOM	2146	NE1	TRP A		50.902	12.233	15.177	1.00 17.37
MOTA	2147		TRP A		49.721	12.862	15.488	1.00 18.60
MOTA	2148	CE3	TRP A		48.911	14.446	17.130	1.00 19.20
MOTA	2149	CZ2	TRP A	331	48.467	12.778	14.874	1.00 17.86
MOTA	2150	CZ3	TRP A	331	47.659	14.364	16.521	1.00 19.94
MOTA	2151	CH2	TRP A	331	47.450	13.535	15.406	1.00 19.08
ATOM	2152	N	GLN A		54.598	13.730	19.873	1.00 23.04
ATOM	2153	CA	GLN A		55.689	14.321		
							20.648	1.00 25.14
ATOM	2154	C	GLN A		55.490	15.836	20.594	1.00 23.64
MOTA	2155	0	GLN A		55.066	16.397	19.533	1.00 23.11
ATOM	2156	CB	GLN A		57.020	13.937	20.015	1.00 27.80
MOTA	2157	ĊG	GLN A	332	58.171	13.877	20.982	1.00 33.30
MOTA	2158	CD	GLN A	332	59.450	13.445	20.305	1.00 35.55
ATOM	2159	OE1	GLN A		60.060	14.224	19.507	1.00 36.94
ATOM	2160		GLN A		59.879	12.217	20.579	1.00 36.57
ATOM	2161	NEZ	ALA A		55.778			
						16.506	21.704	1.00 22.79
ATOM	2162	CA	ALA A		55.618	17.977	21.820	1.00 21.04
ATOM	2163	С	ALA A		55.936	18.759	20.552	1.00 19.77
ATOM	2164	0	ALA A		57.076	18.671	19.997	1.00 19.85
MOTA	2165	CB	ALA A	333	56.475	18.499	22.971	1.00 21.00
MOTA	2166	N	GLY A	334	54.949	19.515	20.083	1.00 17.64

	MOTA	2167	CA	GLY A	334	,	55.123	20.340	18.903	1.00 16.89
	MOTA	2168	С	GLY A			55.205	19.663	17.548	1.00 17.61
	АТОМ		. 0	GLY A			55.403	20.370	16.512	1.00 17.50
	ATOM	2170	N	THR À			55.060	18.343	17.490	1.00 16.55
	ATOM	2171	CA	THR A			55.146	17.648	16.182	1.00 10.55
	ATOM	2172	C	THR A			53.802	17.260	15.557	1.00 17.38
									14.618	
	ATOM	2173	0	THR A			53.761	16.408		1.00 17.71
	ATOM	2174	CB	THR A			56.017	16.377	16.275	1.00 17.76
	ATOM	2175	OG1	THR A		~ .	55.361	15.401	17.095	1.00 17.56
	ATOM	2176	CG2	THR A			57.373	16.710	16.884	1.00 17.23
	ATOM	2177	И	THR A			52.707	17.842	16.037	1.00 16.75
	ATOM	2178	CA	THR A			51.373	17.527	15.460	1.00 16.56
	ATOM.	2179 ·	C	THR A			51.473	17.752		1.00 16.24
	ATOM	2180	0	THR A	336		51.821	18.868	13.487	1.00 16.30
	MOTA	2181	CB	THR A	336		50.267	18.437	16.030	1.00 17.05
	MOTA	2182	OG1	THR A	336		50.181	18.255	17.451	1.00 17.15
	ATOM	2183	CG2	THR A	336		48.917	18.096	15.401	1.00 16.72
	ATOM	2184	N	PRO A	337		51.182	16.718	13.157	1.00 15.50
	ATOM	2185	CA	PRO A	337		51.254	16.820	11.699	1.00 14.87
	ATOM	2186	С	PRO A	337		50.006	17.444	11.082	1.00 14.56
	ATOM	2187	O-	PRO A	337		49.310	16.800	10.249	1.00 14.49
	ATOM	2188	CB	PRO A	337		51.448	15.369	11.281	1.00 15.18
	ATOM	2189	CG	PRO A	337		50.520	14.657	12.238	1.00 16.05
•	MOTA	2190	CD	PRO A	337		50.784	15.359	13.572	1.00 15.54
	MOTA	2191	N	TRP A	338		49.713	18.682	11.470	1.00 14.89
	MOTA	2192	CA	TRP A	338		48.535	19.415	10.956	1.00 14.85
	ATOM	2193	С	TRP A	338		48.339	19.304	9.445	1.00 14.87
	MOTA	2194	0	TRP A	338		47.194	19.048	8.966	1.00 17.13
	ATOM	2195	CB	TRP A	338		48.639	20.899	11.313	1.00 13.77
	ATOM	2196	CG	TRP A			48.784	21.176	12.767	1.00.15.11
	ATOM	2197	CD1	TRP A	338		49.897	21.652	13.411	1.00 14.78
	MOTA	2198	CD2	TRP A			47.780	21.011	13.771	1.00 14.17
	ATOM	2199	NE1	TRP A	338		49.641	21.794	14.756	1.00 14.64
	ATOM :	2200	CE2	TRP A			48.348	21.407	15.003	1.00 14.35
	ATOM	2201	CE3	TRP A			46.451	20.566	13.751	1.00 14.31
	ATOM	2202	CZ2	TRP A			47.635	21.371	16.202	1.00 14.86
		2203	CZ3	TRP A	338		45.744	20.530	14.945	1.00 16.02
	ATOM	2204	CH2	TRP A			46.339	20.932	16.154	1.00 14.77
	ATOM ·	2205	N	ASN A		•	49.414	19.486	8.682	1.00 13.22
	MOTA	2206	CA	ASN A	339		49.319	19.449	7.203	1.00 12.87
	ATOM ·	2207	С	ASN A		-	48.674	18.208	6.608	1.00 12.01
	ATOM		0	ASN A			48.061	18.288		1.00 13.99
	ATOM	2209	СВ	ASN A			50.699	19.649	6.552	1.00 12.61
	ATOM	2210	CG	ASN A			51.576	18.404	6.627	1.00 15.28
	MOTA	2211	OD1	ASN A			52.290		7.648	1.00 16.29
	MOTA	2212		ASN A			51.541	17.584	5.578	1.00.12.93
	ATOM	2213	N	ILE A			48.774	17.064	7.276	1.00 12.88
	MOTA	2214	CA	ILE A			48.171	15.831	6.698	1.00 12.98
	ATOM	2215	C.	ILE A			46.655		6.794	1.00 12.80
	ATOM	2216		ILE A			45.944		5.959	1.00 12.80
	ATOM	2217	СВ	ILE A			48.667		7.400	1.00 14.79
	ATOM	2218	CG1				48.142	14.512	8.833	1.00 14.91
	ATOM	2219	CG2	ILE A			50.194	14.483	7.372	1.00 12.38
	MOTA	2220		ILE A			48.177	13.142	9.454	1.00 17.42
	ATOM	2221	N	PHE A			46.138	16.577	7.790	1.00 13.19
	ATOM	2222	CA	PHE A			44.677		7.972	1.00 13.13
	ATOM	2223	C	PHE A			44.143	17.741	7.006	1.00 13.37
	MOTA	2224		PHE A			44.787		6.798	1.00 13.37
	ATOM	2225		-PHE A			44.767		9.410	1.00 12.72
	ATOM	2225	СĞ	PHE A			44.334		10.429	1.00 13.10
	ATOM			PHE A			44.885		10.425	1.00 13.33
	ATOM	2227		PHE A		•		16.104		1.00 13.48
	AIOM	2228	CD2	rne A	. J-4-T		45.861	TO.TO4.	11.11	1.00 14.14

ATOM	2229	CEl	PHE A	341	44.115	13.984	11.607	1.00 13.44
ATOM	2230	CE2	PHE A	341	46.172	15.136	12.127	1.00 14.31
ATOM	2231	CZ	PHE A		45.298	14.074	12.346	1.00 13.92
	•							
ATOM	2232	N	PRO A		42.975	17.484	6.402	1.00 12.78
MOTA	2233	CA	PRO A	342	42.357	18.413	5.448	1.00 12.17
MOTA	2234	С	PRO A	342	41.565	19.544	6.100	1.00 12.90
ATOM	2235	0	PRO A		41.168	19.465	7.309	1.00 12.52
	2236	СB	PRO A					
ATOM					41.447	17.502	4.638	1.00 10.18
MOTA	2237	CG	PRO A		40.920	16.570	5.714	1.00 11.48
ATOM	2238	CD	PRO A	342	42.180	16.244	6.523	1.00 12.10
MOTA	2239	N	VAL A	343	41.342	20.609	5.342	1.00 12.27
MOTA	2240	CA	VAL A		40.528	21.712	5.851	1.00 10.51
ATOM	2241	C	VAL A		39.101	21.281	5.521	
MOTA	2242	0	VAL A		38.878	20.401	4.632	1.00 10.45
MOTA	2243	CB	VAL A	343	40.838	23.054	5.143	1.00 10.23
MOTA	2244	CG1	VAL A	343	42.247	23.507	5.488	1.00 8.58
ATOM	2245	CG2	VAL A	343	40.672	22.914	3.636	1.00 8.08
ATOM	2246	N	ILE A		38.132	21.848	6.224	1.00 13.49
	2247	CA	ILE A		36.725	21.507	5.991	
MOTA								
MOTA	2248	С	ILE A		35.989	22.789	5.664	1.00 13.33
MOTA	2249	0	ILE A	344	36.067	23.795	6.427	1.00 13.12
MOTA	2250	CB	ILE A	344	36.099	20.859	7.246	1.00 14.77
ATOM	2251	CG1	ILE A	344	36.776	19.512	7.517	1.00 14.50
ATOM	2252	CG2	ILE A		34.585	20.702	7.060	1.00 13.14
	2253	CD1						
MOTA			ILE A		36.374	18.875	8.825	1.00 17.73
MOTA	2254	N	SER A		35.292	22.794	4.537	1.00 12.41
MOTA	2255	CA	SER A	345	34.547	23.982 ·	4.136	1.00 13.41
MOTA	2256	С	SER A	345	33.051	23.723	4.172	1.00 14.94
MOTA	2257	0	SER A	345	32.555	22.641	3.721	1.00 14.55
ATOM	2258	СВ	SER A		34.967	24.430	2.728	1.00 14.23
MOTA	2259	OG	SER A		36.329	24.834	2.703	1.00 13.57
MOTA	2260	N	LEU A	346	32.320	24.682	4.725	1.00 13.42
MOTA	2261	CA	LEU A	346	30.859	24.594	4.796	1.00 14.08
ATOM	2262	С	LEU A	346	30.320	25.772	4.003	1.00 13.86
ATOM	2263	0	LEU A		30.681	26.956	4.286	1.00 13.52
	2264	СB	LEU A		30.383	24.674	6.252	1.00 15.83
ATOM								
MOTA	2265	CG	LEU A		30.239	23.372	7.051	1.00 17.74
MOTA	2266	CD1	LEU A		31.455	22.492	6.875	1.00 18.92
MOTA	2267	CD2	LEU A	346	30.028	23.711	8.521	1.00 19.69
MOTA	2268	N	TYR A	347	29.496	25.485	3.000	1.00 13.48
ATOM	2269	CA	TYR A	347	28.894	26.543	2.176	1.00 13.76
ATOM	2270	C	TYR A		27.525	26.864	2.745	1.00 14.58
		_	TYR A					1.00 14.38
MOTA	2271	0			26.676	25.948	2.979	
ATOM	2272	CB	TYR A		28.757	26.101	0.716	1.00 14.82
ATOM	2273	CG	TYR A	347	30.066	26.051	-0.034	1.00 15.10
ATOM	2274	CD1	TYR A	347	31.022	25.074	0.252	1.00 13.97
ATOM	2275	CD2	TYR A	347	30.349	26.977	-1.038	1.00 13.98
ATOM	2276	CE1			32.228	25.018	-0.447	1.00 14.47
	2277	CE2	TYR A					
MOTA					31.556	26.930	-1.746	
ATOM	2278	CZ	TYR A		32.487		1.445	1.00 15.09
ATOM	2279	OH	TYR A		33.672	25.895	-2.141	1.00 16.72
ATOM	2280	N	LEU A	348	27.288	28.145	2.971	1.00 13.86
MOTA	2281	CA	LEU A		26.018	28.593	3.545	1.00 16.70
ATOM	2282	C	LEU A		25.246	29.445	2.559	1.00 17.37
MOTA	2283	0	LEU A			30.183	1.722	1.00 16.05
MOTA	2284	CB	LEU A		26.292	29.401	4.814	1.00 15.57
MOTA	2285	CG	LEU A	348	27.019	28.620	5.908	1.00 17.10
ATOM	2286	CD1	LEU A	348	27.518	29.565	6.985	1.00 15.71
ATOM	2287		LEU A		26.078	27.580	6.495	1.00 16.92
ATOM	2288	N	MET A		23.922	29.352	2.617	1.00 19.68
			MET A					
MOTA	2289	CA			23.073	30.167	1.734	1.00 22.78
MOTA	2290	С	MET A	349	23.384	31.629	2.024	1.00 22.03

			•					
ATOM	2291	0	MET A 349		23.478	32.049	3.222	1.00 20.70
MOTA	2292	СВ	MET A 349		21.594	29.897	2.008	1.00 25.40
ATOM	2293.	CG	MET A 349		20.931	28.954	1.012	1.00 31.18
ATOM	2294	SD	MET A 349		19.139	28.833	1.272	1.00 37.43
ATOM	2295	CE	MET A 349		18.697	30.583	1.318	1.00 37.43
			GLY A 350		23.573	32.414		1.00 32.73
ATOM	2296	N					0.972	
ATOM	2297	CA	GLY A 350		23.857	33.824	1.167	1.00 23.50
ATOM	2298	С	GLY A 350		22.565	34.612	1.280	1.00 24.26
MOTA	2299	0	GLY A 350		21.450	34.042	1.091	1.00 23.13
MOTA	2300	N	GLU A 35		22.662	35.899	1.591	1.00 27.25
ATOM	2301	CA	GLU A 35:		21.448	36.734	1.698	1.00 32.00
MOTA	2302	С	GLU A 35		20.870	36.948	0.306	1.00 33.92
MOTA	2303	0	GLU A 35:	-	19.620	37.066	0.125	1.00 34.42
MOTA	2304	CB	GLU A 35	•	21.774	38.081	2.340	1.00 32.31
MOTA	2305	CG	GLU A 35	-	22.012	37.996	3.831	1.00 34.92
ATOM	2.306	CD	GLU A 35	_	21.916	39.346	4.503	1.00 35.55
MOTA	2307	OE1	GLU A 35	_	22.819	40.187	4.293	1.00 36.64
MOTA	2308	OE2	GLU A 35	<u>.</u>	20.927	39.567	5.233	1.00 36.29
ATOM	2309	N	VAL A 35	2	21.753	37.007	-0.684	1.00 36.98
MOTA	2310	CA	VAL A 35	2	21.327	37.181	-2.082	1.00 38.72
ATOM	2311	C.	-VAL A 35		20.944		-2.629	1.00 40.47
MOTA	2312	0	VAL A 35		21.689	34.799	-2.426	1.00 39.68
ATOM	2313	CB	VAL A 35		22.456	37.767	-2.939	1.00 38.31
ATOM	2314		VAL A 35		21.999	37.892	-4.382	1.00 38.33
ATOM	2315	CG2			22.866	39.123	-2.391	1.00 37.93
MOTA	2316	N	THR A 35		19.806	35.747	-3.314	1.00 42.33
ATOM	2317	CA	THR A 35		19.300	34.476	-3.882	1.00 43.97
ATOM	2318	C	THR A 35		20.254	33.832	-4.877	1.00 43.18
	2319	0	THR A 35		20.234	34.536	-5.688	1.00 42.65
ATOM		CB	THR A 35		17.929	34.672	-4.578	1.00 45.29
MOTA	2320				18.018	35.743	-5.526	1.00 45.29
ATOM	2321	OG1	THR A 35				-3.551	1.00 46.31
MOTA	2322	CG2			16.849	34.988		
MOTA	2323	N	ASN A 35		20.307	32.507	-4.839	1.00 42.20
ATOM	2324	CA	ASN A 35		21.183	31.741	-5.742	1.00 43.39
MOTA	2325	Ç	ASN A 35		22.641	32.166	-5.611	1.00 41.22
MOTA	2326	0	ASN A 35		23.444	32.078	-6.584	1.00 43.04
MOTA	2327	СВ	ASN A 35		20.698	31.887	-7.187	1.00 45.64
MOTA	2328	CG	ASN A 35		19.467	31.036		1.00 47.44
ATOM	2329	OD1	ASN A 35		18.824	31.163	-8.562	1.00 48.61
MOTA	2330	ND2			19.121	30.159	-6.534	1.00 47.73
MOTA	2331	N	GLN A 35		22.999	32.621	-4.419	1.00 37.62
MOTA	2332	CA	GLN A 35			33.042	-4.128	1.00 34.85
MOTA	2333	С	GLN A 35		24.737	32.475	-2.764	1.00 32.57
ATOM	2334	0	GLN A 35	5	23.863	32.388	-1.846	1.00 31.25
MOTA	2335	CB	GLN A 35	5	24.459	34.563	-4.105	1.00 35.77
MOTA	2336	CG	GLN A 35	5	25.834	35.089		1.00 38.04
ATOM	2337	CD	GLN A 35	5	25.909	36.590	-3.915	1.00 39.05
MOTA	2338	OE1	GLN A 35	5 .	25.586	37.171	-4.992	1.00.40.57
ATOM	2339	NE2	GLN A 35	5	26.331	37.249	-2.844	1.00 39.68
ATOM	2340	N	SER A 35	6	25.989	32.071	-2.597	1.00 29.33
ATOM	2341	CA	SER A 35		26.419	31.514	-1.304	1.00 25.60
ATOM	2342	С	SER A 35		27.850	31.897	-0.981	1.00 22.66
ATOM	2343	Ö	SER A 35		28.580	32.481	-1.833	1.00 21.99
MOTA	2344	СB	SER A 35		26.313	29.991	1.318	1.00 25.71
MOTA			SER A 35		27.449	29.425	-1.945	1.00 24.59
	2346	N	PHE A 35		28.267	31.583		1.00 20.53
ATOM	2347	CA	PHE A 35		29.639	31.865	0.676	1.00 17.95
ATOM	2348		PHE A 35		30.104	30.643	1.437	1.00 17.15
	2349	Ö	•		29.279	29.750	1.784	1.00 17.13
ATOM			PHE A 35			33.126	1.754	1.00 17.21
ATOM.	2350	CB	PHE A 35		29.687		2.850	1.00 17.62
ATOM	2351	CG	PHE A 35		28.926	33.017	4.018	1.00 17.81
ATOM	2352	CDI	PHE A 35	7	29.571	32.625	#.OTQ	T.00 T.03

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\mathtt{ATOM}	2353	CD2	PHE A	357	27.577	33.357	2.912	1.00 16.90
MOTA	2354	CE1	PHE A	357	28.887	32.577	5.229	1.00 14.87
MOTA		CE2	PHE A		26.881	33.312	4.120	
	2355.							1.00 15.64
MOTA	2356	CZ	PHE A		27.538	32.924	5.280	1.00 16.14
MOTA	2357	N	ARG A	358	31.397	30.545	1.687	1.00 16.29
ATOM	2358	CA	ARG A		31.891	29.383	2.412	1.00 14.04
ATOM	2359	C	ARG A		32.642	29.755	3.664	1.00 14.59
ATOM	2360	0	ARG A	358	33.237	30.869	3.785	1.00 13.01
ATOM	2361	СВ	ARG A		32.784	28.525	1.516	1.00 14.11
								_
MOTA	2362	CG	ARG A	358	34.084	29.172	1.102	1.00 13.28
ATOM	2363	CD	ARG A	358	34.809	28.275	0.121	1.00 13.06
ATOM	2364	NE	ARG A		36.090	28.831	-0.291	1.00 14.39
								_
ATOM	2365	CZ	ARG A		36.723	28.489	-1.409	1.00 14.92
ATOM	2366	NH1	ARG A	358	36.188	27.591	-2.232	1.00 13.71
ATOM	2367	NH2	ARG A	358	37.888	29.045	-1.701	1.00 12.88
					32.612		4.596	
ATOM	2368	И	ILE A			28.819		1.00 14.51
ATOM	2369	CA	ILE A	359	33.268	28.935	5.891	1.00 16.36
ATOM	2370	С	ILE A	359	34.242	27.762	5.913	1.00 15.41
ATOM	2371	0	ILE A		33.836	26.583	5.675	1.00 15.49
ATOM	2372	CB	ILE A		32.197	28.824	7.001	1.00 17.94
ATOM	2373	CG1	ILE A	359	31.543	30.190	7.198	1.00 19.68
ATOM	2374	CG2	ILE A	359	32.766	28.260	8.255	1.00 20.12
ATOM	2375	CD1	ILE A		32.515	31.288	7.500	1.00 22.40
MOTA	2376	N	THR A	360	35.513	28.046	6.162	1.00 13.01
ATOM	2377	CA	THR A	360	36.531	26.983	6.167	1.00 14.32
ATOM	2378	С	THR A		37.307	26.894	7.470	1.00 14.04
ATOM	2379	. 0	THR A		37.892	27.913	7.938	1.00 13.82
MOTA	2380	CB	THR A	360	37.536	27.202	5.021	1.00 14.49
ATOM	2381	0G1	THR A	360	36.828	27.286	3.774	1.00 15.69
		CG2			38.532	26.053	4.964	1.00 15.11
MOTA	2382		THR A					
ATOM	2383	N	ILE A	361	37.331	25.709	8.074	1.00 13.79
ATOM	2384	CA	ILE A	361	38.091	25.524	9.330	1.00 17.36
ATOM	2385	C	ILE A	361	39.241	24.548	9.122	1.00 16.53
MOTA	2386	0	ILE A		39.237	23.717	8.160	1.00 16.37
MOTA	2387	CB	ILE A	361	37.208	24.982	10.476	1.00 18.15
ATOM	2388	CG1	ILE A	361	36.608	23.632	10.077	1.00 18.53
ATOM	2389	CG2	ILE A		36.126	25.999	10.830	1.00 18.95
\mathtt{ATOM}	2390	CD1	ILE A	361	35.899	22.937	11.208	1.00 18.19
ATOM	2391	N	LEU A	362	40.230	24.614	9.998	1.00 17.82
ATOM	2392	CA	LEU A	362	41.375	23.710	9.876	1.00 18.92
					41.412		10.983	1.00 17.87
ATOM	2393	С	LEU A			22.659		
ATOM	2394	0	LEU A	362	40.533	22.654	11.912	1.00 17.21
MOTA	2395	CB	LEU A	362	42.675	24.525	9.837	1.00 22.47
ATOM	2396	CG	LEU A		42.686	25.974	10.320	1.00 25.03
					42.945	25.992	11.802	1.00 28.14
MOTA	2397		LEU A					
MOTA	2398	CD2	LEU A	362	43.781	26.751	9.623	1.00 25.06
MOTA	2399	N	PRO A	363	42.380	21.729	10.910	1.00 16.12
MOTA	2400	CA	PRO A		42.507	20.681	11.925	1.00 14.51
MOTA	2401	C	PRO A		42.628	21.325	13.303	1.00 14.50
ATOM	2402	0	PRO A	363	42.234	20.710	14.339	1.00 13.48
ATOM	2403	CB	PRO A	363	43.801	19.971	11.534	1.00 15.57
ATOM	2404	CG	PRO A		43.902	20.202	10.076	1.00 16.87
ATOM	2405	CD	PRO A		43.450	21.616	9.903	1.00 14.60
ATOM	2406	N	GLN A	364	43.178	22.539	13.337	1.00 12.36
ATOM		CA	GLN A		43.357	23.271	14.608	1.00 13.04
	2407							
MOTA	2408	C	GLN A		42.014	23.557	15.254	1.00 13.41
ATOM	2409	0	GLN A	364	41.953	23.895	16.467	1.00 12.73
ATOM	2410	CB	GLN A		44.111	24.585	14.392	1.00 12.04
			GLN A				14.304	1.00 11.85
ATOM	2411	CG			45.637	24.449		
MOTA	2412	CD	GLN A		46.141	24.079	12.919	1.00 11.11
ATOM	2413	OE1	GLN A	364	47.372	24.211	12.625	1.00 13.65
ATOM	2414		GLN A		45.245	23.621	12.056	1.00 8.04
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MOTA 2415 N GLN A 365 40.939 23.446 14.478 1.00 13.30 39.580 23.657 15.023 GLN A 365 1.00 14.36 MOTA 2416 CA 38.873 22.341 15.339 1.00 14.57 GLN A 365'. 2417 С MOTA 38.312 22.175 16.457 1.00 16.56 MOTA 2418 0 . GLN A 365 38.691 24.452 14.056 MOTA 2419 CB GLN A 365

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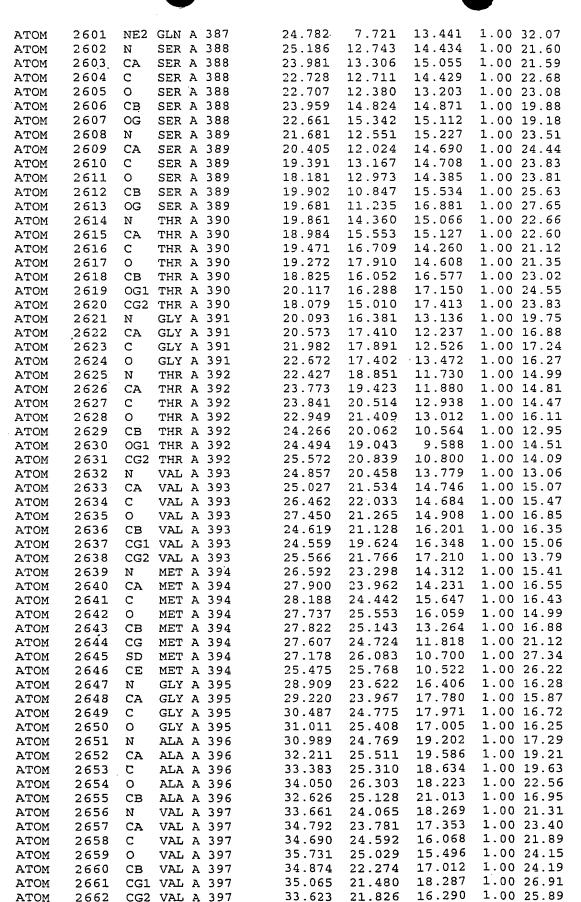
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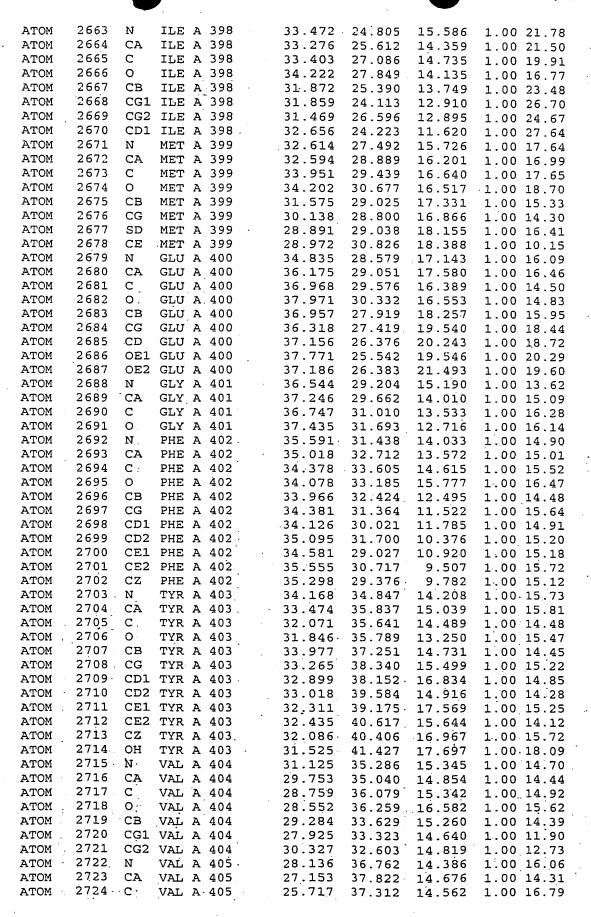
 1.00 14.03 GLN A 365 MOTA 2420 CG GLN A 365 CD MOTA 2421 OE1 GLN A 365 MOTA 2422 NE2 GLN A 365 MOTA 2423 TYR A 366 MOTA 2424 N CA TYR A 366 ATOM 2425 TYR A 366 2426 C ATOM TYR A 366 MOTA 2427 0 2428 CB TYR A 366 ATOM TYR A 366 ATOM. 2429 CG 2430 CD1 TYR A 366 MOTA 2431 CD2 TYR A 366 MOTA 40.062 17.431 11.463 1.00 12.91 39.555 19.369 10.128 1.00 12.63 40.218 18.163 10.294 1.00 13.86 41.008 17.669 9.287 1.00 12.42 ATOM 2432 CE1 TYR A 366 MOTA 2433 CE2 TYR A 366 CZ TYR A 366 MOTA 2434 2435 OH TYR A 366 MOTA 40.144 19.367 15.835 1.00 16.84 LEU A 367 ATOM 2436 N 40.966 18.450 16.660 1.00 16.98 40.996 19.161 18.017 1.00 17.50 41.662 20.224 18.172 1.00 16.40 CA LEU A 367 MOTA 2437 LEU A 367 ATOM 2438 C LEU A 367 ATOM 2439 0 42.382 18.324 16.088 1.00 17.44 2440 CB LEU A 367 MOTA 42.764 16.991 15.429 1.00 18.54 2441 CG LEU A 367 MOTA 41.681 16.534 14.482 1.00 17.60 44.091 17.143 14.700 1.00 17.38 CD1 LEU A 367 MOTA 2442 MOTA 2443 CD2 LEU A 367 40.270 18.624 18.990 1.00 17.06 2444 N. ARG A 368 ATOM 40.192 19.253 20.326 1.00 17.22 2445 CA ARG A 368 MOTA 41.341 18.874 21.243 1.00 16.52 ARG A 368 MOTA 2446 C 41.554 17.662 21.538 1.00 16.52 41.554 17.662 21.538 1.00 16.19 38.879 18.871 21.009 1.00 16.02 38.050 20.055 21.444 1.00 19.09 37.415 19.811 22.792 1.00 17.88 36.840 18.474 22.906 1.00 17.20 ARG A 368 MOTA 2447 0 2448 CB ARG A 368 MOTA MOTA 2449 CG ARG A. 368 CD ARG A 368 MOTA 2450 NE ARG A 368 MOTA 2451 36.775 17.806 24.053 1.00 18.65 37.247 18.361 25.164 1.00 18.77 CZ ARG A 368 MOTA 2452 NH1 ARG A 368 MOTA 2453 36.258 16.584 24.095 1.00 17.53 ATOM 2454 NH2 ARG A 368 42.100 19.867 21.722 1.00 17.88 PRO A 369 ATOM 2455 N 43.220 19.558 22.615 1.00 19.69 MOTA 2456 CA PRO A 369 42.744 19.067 23.969 1.00 22.16 41.786 19.645 24.575 1.00 20.49 43.983 20.883 22.700 1.00 20.03 PRO A 369 ATOM · 2457 С PRO A 369 MOTA 2458 0 CB PRO A 369 MOTA 2459 42.932 21.911 22.429 1.00 19.96 42.122 21.285 21.320 1.00 19.96 43.376 18.001 24.444 1.00 23.75 ATOM 2460 CG PRO A 369 CD PRO A 369 MOTA 2461 VAL A 370 ATOM 2462 N 43.040 17.399 25.747 1.00 27.84 2463 CA VAL A 370 MOTA 44.332 16.921 26.394 1.00 30.26 45.321 16.577 25.682 1.00 30.79 42.093 16.197 25.577 1.00 26.52 40.771 16.654 24.989 1.00 26.57 42.737 15.160 24.669 1.00 26.53 VAL A 370 ATOM 2464 C ATOM 2465 O VAL A 370 2466 CB VAL A 370 ATOM CG1 VAL A 370 2467 ATOM -ATOM 2468 CG2 VAL A 370 44.361 16.891 27.719 1.00 35.50 45.574 16.450 28.426 1.00 40.60 ATOM · 2469 GLU A 371 N ATOM: 2470 CA GLU A 371 45.574 16.450 28.426 1.00 40.60 45.800 14.963 28.235 1.00 42.42 44.832 14.138 28.321 1.00 41.89 45.472 16.758 29.921 1.00 43.12 GLU A 371 ATOM: 2471 С GLU A 371 ATOM 2472 0 CB GLU A 371 ATOM : 2473 46.603 17.634 30.443 1.00 47.33 47.954 17.245 29.864 1.00 49.98 48.264 16.036 29.818 1.00 51.63 ATOM 2474 CG GLU A 371 2475 CD GLU A 371 ATOM 2476 OE1 GLU A 371 MOTA

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ATOM	2477	OE2	GLU A	371	48.710	18.151	29.456	1.00 51.00
ATOM	2478	N	ASP A		47.046	14.596	27.960	1.00 45.77
MOTA	2479.	CA	ASP A		47.396	13.182	27.774	1.00 49.75
MOTA	2480	С	ASP A	372	46.889	12.468	29.014	1.00 52.41
ATOM	2481	0	ASP A	372	47.090	12.966	30.165	1.00 52.32
ATOM	2482	CB	ASP A		48.913	13.015	27.665	1.00 50.28
MOTA	2483	CG	ASP A		49.323	11.587	27.333	1.00 51.15
MOTA	2484	OD1	ASP A	x 372	50.541	11.323	27.246	1.00 51.32
ATOM	2485	OD2	ASP A	372	48.429	10.729	27.156	1.00 50.76
ATOM	2486	N	VAL A		46.217	11.340	28.819	1.00 55.35
ATOM	2487	CA	VAL A		45.688	10.570	29.956	
								1.00 58.73
MOTA	2488	С	VAL A		46.850	10.213	30.896	1.00 60.04
ATOM	2489 ·	0	VAL A	373	47.465	9.105	30.817	1.00 60.06
MOTA	2490	CB	VAL A	373	44.901	9.313	29.433	1.00 59.43
MOTA	2491	CG1	VAL A		45.292	8.044	30.176	1.00 59.64
ATOM	2492	CG2	VAL A		43.402	9.556	29.597	1.00 59.89
MOTA	2493	N	ALA A		47.187	11.169	31.759	1.00 61.58
ATOM	2494	CA	ALA A	374	48.277	11.020	32.755	1.00 61.52
MOTA	2495	С	ALA A	374	49.709	11.205	32.233	1.00 61.38
ATOM	2496	0	ALA A	374	50.104	10.633	31.169	1.00 60.95
ATOM	2497	CB	ALA A		48.155	9.668	33.455	1.00 62.66
MOTA	2498	N	THR A		50.477	12.002	32.977	1.00 61.03
ATOM	2499	CA	THR A	375	51.919	12.320	32.715	1.00 60.30
ATOM	2500	C	THR A	375	52.401	12.358	31.269	1.00 58.41
MOTA	2501	0	THR A	375	52.361	11.308	30.555	1.00 59.21
ATOM	2502	СВ	THR A		52.838	11.327	33.455	1.00 61.35
			THR A					
MOTA	2503				52.302	11.049	34.756	1.00 62.26
ATOM	2504	CG2	THR A		54.237	11.912	33.599	1.00 61.47
MOTA	2505	N	SER A	376	52.892	13.520	30.833	1.00 55.18
ATOM	2506	CA	SER A	376	53.407	13.683	29.445	1.00 51.40
ATOM	2507	С	SER A		53.538	15.132	28.981	1.00 48.79
MOTA	2508	Õ	SER A		52.887	16.067	29.540	1.00 48.19
MOTA	2509	CB	SER A		52.502	12.943	28.456	1.00 51.90
ATOM	2510	OG	SER A	376	52.880	13.193	27.115	1.00 51.94
MOTA	2511	N	GLN A	377	54.373	15.333	27.968	1.00 44.88
MOTA	2512	CA	GLN A	377	54.576	16.664	27.367	1.00 41.28
ATOM	2513	C	GLN A		54.106	16.580	25.923	1.00 37.22
MOTA	2514	0	GLN A		54.380	17.489	25.081	1.00 35.23
MOTA	2515	CB	GLN A		56.048	17.062	27.425	1.00 43.59
MOTA	2516	CG	GLN A	377	56.468	17.585	28.789	1.00 46.22
ATOM	2517	CD	GLN A	377	57.955	17.831	28.886	1.00 47.12
MOTA	2518	OE1	GLN A	377	58.710	17.710	27.867	1.00 48.44
ATOM	2519		GLN A		58.414	18.177	30.081	1.00 48.23
MOTA	2520	N	ASP A		53.399	15.499	25.618	1.00 31.89
MOTA	2521	CA	ASP A	378	52.866	15.289	24.263	1.00 28.31
ATOM	2522	C	ASP A	378	51.663	16.183	24.034	1.00 25.36
MOTA	2523	0	ASP A	378	50.958	16.590	25.004	1.00 22.58
MOTA	2524	CB	ASP A		52.422	13.835	24.072	1.00 28.64
MOTA	2525	CG	ASP A		53.582	12.867	23.998	1.00 29.19
MOTA	2526	OD1	ASP A	378	54.746	13.316	23.948	1.00 30.91
ATOM	2527	OD2	ASP A	378	53.323	11.647	23.981	1.00 30.50
MOTA	2528	N	ASP A		51.415	16.513	22.776	1.00 23.06
MOTA	2529	ĊA	ASP A		50.236	17.317	22.436	1.00 22.51
								1.00 22.31
ATOM	2530	C	ASP A	•	49.220	16.294	21.964	
MOTA	2531	0	ASP A		49.436	15.581	20.945	1.00 19.87
ATOM	2532	CB	ASP A	379	50.570	18.335	21.346	1.00 21.72
MOTA	2533	CG	ASP A	379	51.557	19.377	21.829	1.00 23.29
MOTA	2534		ASP A		51.434	19.786	23.005	1.00 23.00
ATOM	2535		ASP A		52.446	19.789	21.052	1.00 23.50
MOTA	2536	N	CYS A		48.128		22.706	1.00 20.99
ATOM	2537	CA	CYS A		47.082	15.201	22.393	1.00 20.40
MOTA	2538	С	CYS A	380	45.769	15.865	22.013	1.00 19.94

ATOM	2539	0	CYS A .380		45.489	17.038	22.417	-1.00 18.77
ATOM	2540	СB	CYS A 380		46.867	14.292	23.596	1.00 23.14
MOTA	2541	SG	CYS A 380		48.368	13.550	24.327	1.00 25.25
ATOM	2542	N	TYR A 381		44.947	15.140	21.255	1.00 18.49
ATOM :	2543	CA	TYR A 381		43.656	15.681	20.785	1.00 17.31
MOTA	2544	C	TYR A 381		42.595	14.610	20.602	1.00 17.31
ATOM	2545	0	TYR A 381		42.890	13.376	20.532	1.00 17.45
ATOM	2546	CB	TYR A 381		43.833	16.370	19.427	1.00 15.47
ATOM	2547	CG	TYR A 381		45.034	17.275	19.314	1.00 13.47
ATOM	2548	CD1	TYR A 381		44.899	18.659	19.408	1.00 14.33
ATOM	2549	CD2	TYR A 381		46.311	16.746	19.118	1.00 14.17
ATOM	2550	CE1	TYR A 381		46.009	19.499	19.307	1.00 14.17
ATOM	2551	CE2	TYR A 381		47.431	17.576	19.021	1.00 14.00
ATOM	2552	CZ	TYR A 381		47.272	18.952	19.113	1.00 16.02
MOTA	2553	OH	TYR A 381		48.369	19.785	18.994	1.00 15.32
ATOM	2554	N	LYS A 382		41.356	15.765	20.506	1.00 18.35
ATOM	2555	CA	LYS A 382		40.218	14.174	20.248	1.00 20.26
ATOM	2556	C	LYS 'A 382		39.555	14.695	18.981	1.00 20.20
MOTA	2557	0	LYS A 382		39.575	15.941	18.704	1.00 19.65
ATOM	2558	CB	LYS A 382		39.221	14.204	21.404	1.00 21.74
ATOM	2559	CG	LYS'A 382		39.632	13.348	22.585	1.00 25.42
ATOM	.2560	CD	LYS A 382		38.509	13.266	23.602	1.00 27.59
ATOM	2561	CE	LYS A 382		38.878	12.342	24.759	1.00 29.84
MOTA	2562	NZ	LYS A 382		37.779	12.246	25.761	1.00 31.22
ATOM	2563	N	PHE A 383		38.994	13.786	18.192	1.00 18.55
MOTA	2564	CA	PHE A 383		38.298	14.165	16.942	1.00 16.97
MOTA	2565	C	PHE A 383		36.992	14.823	17.375	1.00 16.22
ATOM	2566	Ö	PHE A 383		36.079	14.138	17.908	1.00 13.73
MOTA	2567	CB	PHE A 383		38.026	12.907	16.110	1.00 16.57
ATOM	2568	CG	PHE-A 383		37.447	13.182	14.750	1.00 16.49
MOTA	2569		PHE A 383		38.052	14.091	13.890	1.00 14.48
MOTA	2570		PHE A 383		36.319	12.489	14.308	1.00 15.06
ATOM	2571		PHE A 383		37.542	14.306	12.606	1.00 16.02
MOTA	2572	CE2			35.807	12.696	13.029	1.00 15.64
MOTA	2573	CZ	PHE A 383		36.419	13.603	12.176	1.00 15.10
MOTA	2574	N	ALA A 384		36.885	16.134	17.173	1.00 16.28
ATOM	2575	ĊA	ALA A 384		35.675	16.893	17.586	1.00 15.54
MOTA	2576	С	ALA A 384		34.549,		16.559	1.00 15.46
ATOM	2577	0	ALA A 384		33.768	17.931	16.487	1.00 15.60
ATOM	2578	CB	ALA A 384		36.061	18.316	17.987	1.00 14.96
MOTA	2579	N	ILE A 385		34.451	15.888	15.745	1.00 14.66
ATOM '	2580	CA	ILE A 385		33.356	15.792	14.763	1.00 13.45
MOTA	2581	С	ILE A 385		32.651	14.487	15.093	1.00 14.39
ATOM	2582	0	'ILE A 385		33.303	13.410	15.179	1.00 12.37
MOTA	2583	CB	ILE A 385		33.862	15.724	13.315	1.00 12.54
MOTA	2584	CG1	ILE A 385		34.696	16.959	12.988	1.00 13.08
ATOM	2585	CG2	ILE A 385		32.675	15.655	12.367	1.00 12.56
MOTA	2586	CD1			35.178	17.003	11.549	1.00 10.74
MOTA	2587	N	SER A 386		31.343	14.543	15.297	1.00 14.95
MOTA	2588	CA	SER A 386		30.605	13.319	15.637	1.00 16.99
MOTA	2589	Ç	SER A 386		29.275	13.221	14.918	1.00 17.48
MOTA	2590	Ö	SER A 386		28.795	14.207	14.279	1.00 18.09
MOTA	2591	CB	SER A 386		30.385	13.240	17.151	1.00 16.69
ATOM	2592	0G	SER A 386		29.630	14.345	17.616	1.00 16.81
MOTA.		N	GLN A 387		28.673	12.044	15.016	1.00 19.86
MOTA	2594	CA	GLN A 387		27.384	11.748	14.376	1.00 23.09
MOTA	2595	С	GLN A 387	•	26.209	12.317	15.160	1.00 22.61
MOTA	2596	0	GLN A 387		26.221	12.363	16.427	1.00 22.90
ATOM T	2597	CB	GLN A 387	•	27.222	10.234	14.247	
MOTA		CG	GLN A 387		26.035	9.795	13.411	1.00 28.94
ATOM	2599	.CD	GLN A 387		25.971	8.286		1.00 30 39
MOTA	2600	OE1	GLN A 387		27.013	7.619	12.999	1.00 31.54

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ATOM	2725	0	VAL A	405	25.238	36.955	13.443	1.00 16.14
MOTA	2726	CB	VAL A	405	27.318	39.004	13.700	1.00 13.66
	2727		VAL A		26.302	40.092	14.021	1.00 12.39
ATOM								
MOTA	2728	CG2	VAL A	405	28.739	39.547	13.775	1.00 10.80
ATOM	2729	N	PHE A	406	25.019	37.260	15.691	1.00 16.73
ATOM	2730	CA	PHE A	406	23.616	36.805	15.685	1.00 16.71
ATOM	2731	C	PHE A		22.755	38.049	15.531	1.00 17.47
ATOM	2732	0	PHE A		22.286	38.654	16.539	1.00 17.39
MOTA	2733	CB	PHE A	406	23.287	36.053	16.979	1.00 13.96
ATOM	2734	CG	PHE A	406	24.061	34.765	17.139	1.00 13.82
ATOM	2735	CD1	PHE A		25.398	34.783	17.533	1.00 13.31
	2736		PHE A		23.464	33.538	16.863	1.00 12.85
ATOM					=			
MOTA	2737	CEI	PHE A		26.128	33.601	17.646	1.00 13.23
ATOM	2738	CE2	PHE A	406	24.185	32.350	16.973	1.00 12.78
ATOM	2739	CZ	PHE A	406	25.522	32.382	17.367	1.00 12.96
ATOM	2740	N	ASP A	407	22.566	38.449	14.278	1.00 18.08
ATOM	2741	CA	ASP A		21.785	39.647	13.932	1.00 19.70
							13.927	1.00 19.73
ATOM	2742	С	ASP A		20.297	39.316		
ATOM	2743	0	ASP A		19.675	39.120	12.837	1.00 18.96
MOTA	2744	CB	ASP A	407	22.221	40.153	12.552	1.00 22.61
ATOM	2745	CG	ASP A	407	21.663	41.530	12.223	1.00 24.28
ATOM	2746	OD1	ASP A	407	20.660	41.935	12.849	1.00 24.12
	2747		ASP A		22.225	42.198	11.325	1.00 23.37
ATOM								
MOTA	2748	N	ARG A		19.709	39.245	15.116	1.00 19.72
ATOM	2749	CA	ARG A	408	18.269	38.928	15.259	1.00 22.01
MOTA	275 0	С	ARG A	408	17.393	39.967	14.557	1.00 21.56
ATOM	2751	0	ARG A	408	16.386	39.606	13.875	1.00 20.49
ATOM	2752	СB	ARG A		17.909	38.835	16.748	1.00 23.44
					18.670	37.724	17.479	1.00 25.61
MOTA	2753	CG	ARG A					
MOTA	2754	CD	ARG A		18.838	37.994	18.973	1.00 28.14
ATOM	2755	NE	ARG A	408	17.843	37.328	19.814	1.00 31.17
ATOM	2756	CZ	ARG A	408	16.567	37.679	19.887	1.00 32.24
ATOM	2757	NH1	ARG A	408	16.127	38.693	19.163	1.00 35.70
ATOM	2758	NH2	ARĠ A		15.735	37.029	20.687	1.00 31.13
						41.241	14.694	1.00 21.10
MOTA	2759	N	ALA A		17.750			
MOTA	2760	CA	ALA A	409	16.978	42.329	14.056	1.00 22.43
MOTA	2761	C	ALA A	409	16.785	42.050	12.571	1.00 22.80
MOTA	2762	0	ALA A	409	15.646	42.177	12.034	1.00 24.04
ATOM	2763	CB	ALA A	409	17.689	43.664	14.247	1.00 20.85
ATOM	2764	N	ARG A		17.858	41.664	11.889	1.00 23.89
			ARG A		17.770	41.374	10.445	1.00 25.07
ATOM	2765	CA						
MOTA	2766	C	ARG A		17.639	39.888	10.119	1.00 24.26
ATOM	2767	0	ARG A	410	17.908	39.461	8.956	1.00 24.63
ATOM	2768	CB	ARG A	410	18.987	41.949	9.724	1.00 26.83
ATOM	2769	CG	ARG A	410	19.025	43.464	9.700	1.00 29.89
MOTA	2770	CD	ARG A		19.326	43.944	8.295	1.00 32.69
ATOM	2771	NE	ARG A		20.590	44.664	8.208	1.00 33.51
MOTA	2772	CZ	ARG A		21.182	44.979	7.062	1.00 34.58
MOTA	2773	NH1	ARG A	410	20.626	44.631	5.907	1.00 33.99
MOTA	2774	NH2	ARG A	410	22.328	45.644	7.068	1.00 35.27
ATOM	2775	N	LYS A	411	17.223	39.091	11.097	1.00 22.77
ATOM	2776	CA	LYS A		17.061	37.630	10.891	1.00 22.97
								1.00 21.80
MOTA	2777	C	LYS A		18.227	37.031	10.104	
MOTA	2778	0	LYS A		18.015	36.309	9.081	1.00 20.39
MOTA	277 9	CB	LYS A	411	15.761	37.335	10.138	1.00 23.53
ATOM	2780	CG	LYS A	411	14.491	37.686	10.886	1.00 27.80
ATOM	2781	CD	LYS A		13.270	37.188	10.121	1.00 30.25
MOTA	2782	CE	LYS A		13.337	35.678	9.890	1.00 31.18
								1.00 34.08
ATOM	2783	NZ	LYS A		12.153	35.163	9.142	
MOTA	2784	N	ARG A		19.449	37.290	10.541	1.00 19.85
MOTA	2785	CA	ARG A		20.607	36.748	9.815	1.00 18.29
MOTA	2786	С	ARG A	412	21.789	36.505	10.736	1.00 18.54
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ATOM	2787	0	ARG A 412	2	1.911	37.137	11.837	1.00	18.56	
MOTA	27,88	CB	ARG A 412	2	1.019	37.714	8.703	1.00	18.72	
MOTA	2789.	CG	ARG A 412		1.571	39.027	9.239	1.00	18.66	
MOTA	2790	CD	ARG A 412		1.941	39.988	8.127	1.00	18.34	
ATOM	2791	NE	ARG A 412		2.560	41.196	8.662	1.00	19.28	
MOTA	2792	CZ	ARG A 412		3.082	42.163	7.916		20.03	
MOTA	2793	NH1	ARG A 412		3.059	42.067	6.591		19.36	
MOTA	2794	NH2	ARG A 412		3.635	43.219	8.496		19.27	
MOTA	2795	N	ILE A 413		2.668	35.606	10.317		17.01	
MOTA	2796	CA	ILE A 413		3.865	35.285	11.103		16.43	
MOTA	2797	C	ILE A 413		5.103	35.576	10.266		16.20	
ATOM	2798	0	ILE A 413		5.213	35.125	9.084		17.17	*
ATOM	2799	CB	ILE A 413		23.855	33.808	11.533		16.02	
MOTA	2800	CG1			22.667	33.562	12.469		13.92 15.95	
ATOM	2801 2802	CG2 CD1	ILE A 413		25.168 22.482	33.458 32.130	12.218 12.862		14.89	
ATOM ATOM	2802	N,	GLY A 414		26.028	36.332	10.841		15.43	
ATOM	2804	CA	GLY A 414		27.243	36.679	10.132		14.42	
ATOM	2805	Ċ	GLY A 414		28.463	35.899	10.585		14.91	
MOTA	2806	0	GLY A 414		28.569	35.463	11.779		12.74	
ATOM	2807	Ŋ	PHE A 415		29.392	35.709	9.656		12.70	
MOTA	2808	CA	PHE A 415		30.638	34.977	9.932		14.84	*
ATOM	2809	C	PHE A 415		31.823	35.766	9.403		15.05	
MOTA	2810	0	PHE A 415	3	31.761	36.376	8.291	1.00	17.34	
ATOM	2811	CB	PHE A 415	3	30.613	33.599	9.256	1.00	13.57	٠. ٠
ATOM	2812	CG	PHE A 415	2	29.628	32.640	9.860		13.35	
MOTA	2813	CD1	PHE A 415		30.034	31.710	10.820		14.56	
MOTA	2814	CD2			28.296	32.660	9.472		11.54	
MOTA	2815	CE1			29.117	30.809	11.383		13.74	
MOTA	2816	CE2			27.373	31.768	10.027		12.67	
MOTA	2817	CZ	PHE A 415		27.787	30.839	10.985		13.15	
ATOM	2818	N	ALA A 416		32.895	35.779	10.178		15.11	
MOTA	2819.	CA	ALA A 416		34.135	36.470	9.786		14.57	
ATOM ·	2820	C,	ALA A 416		35.248	35.738	10.515		14.48 12.56	-
MOTA	2821 2822	O CB	ALA A 416 ALA A 416		35.027 34.095	35.186 37.935	11.639 10.208		11.46	
MOTA MOTA	2823		VAL A 41		36.425	35.692	9.906		14.71	
ATOM	2824	CA	VAL A 417		37.569	35.011	10.528		16.80	
ATOM	2825	C	VAL A 417		37.835	35.634	11.892		18.08	
ATOM	2826	0.	VAL A 417		37.922	36.901	12.033		17.13	
ATOM	2827		VAL A 41		38.824	35.126	9.642		17.67	
MOTA	2828		VAL A 41		40.022	34.486	10.333		16.83	
ATOM	2829	CG2			38.561	34.441	8.301	1.00	18:32	
MOTA	2830	N.	SER A 418		37.953	34.785	12.905	1.00	17.31	· · · ·
MOTA	2831	CA	SER A 418		38.201	35.271	14.272		17.62	:.
MOTA	2832	C	SER A 418		39.637	35.712	14.455		18.36	
ATOM	2833	· O	SER A 418		40.591	35.038	13.963		19.44	·
ATOM	2834	CB	SER A 418		37.882	34.182	15.295		18.09	
MOTA	2835	OG	SER A 418		38.228	34.617	16.599		17.42	
ATOM	2836	N	ALA A 419		39.821	36.827	. 15.150		17.60	
MOTA	2837	ĊA	ALA A 419		41.175	37.335			18.46	
MOTA	2838	.c	ALA A 419		41.877	36.423	16.423		19.09	
ATOM	2839	0	ALA A 419		43.117	36.553	16.649		19.60	• .
MOTA	2840	CB	ALA A 419		41.106	38.772	15.943		17.70 19.36	
MOTA	2841	N	CYS A 420		41.132	35.500	17.032		20.89	
ATOM	2842 2843	CA	CYS A 420		41.736° 41.677	34.575 33.105	18.029 17.624		19.60	
ATOM ATOM	2843. 2844	С О	CYS A 420		41.805	33.105	18.501		22.74	
ATOM	2845	CB	CYS A 42		41.064	34.734	19.410		21.69	
ATOM	2846	SG	CYS A 42		39.353	34.734	19.526		25.02	
ATOM	2847	N	HIS A 42		41.495	32.814	16.342		17.86	
MOTA	2848	CA	HIS A 42		41.435	31.393	15.933		17.71	
111011		CA	2.	-					_	
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MOTA	2849	С	HIS	A	421	42.834	30.798	15.799	1.00 17.18
ATOM	2850	Ō	HIS			43.801	31.495	15.356	1.00 14.17
ATOM	2851	СВ	HIS			40.641	31.236	14.625	1.00 14.17
MOTA	2852	CG	HIS			41.433	31.504		1.00 18.03
ATOM	2853		HIS			42.114	30.514	12.705	
									1.00 18.84
ATOM	2854		HIS			41.631	32.645	12.678	1.00 18.73
ATOM	2855		HIS			42.695	31.032	11.637	1.00 17.98
ATOM	2856		HIS			42.418	32.323	11.597	1.00 20.03
ATOM	2857	N	VAL			42.965	29.533	16.194	1.00 16.96
MOTA	2858	CA	VAL			44.260	28.816	16.132	1.00 16.89
ATOM	2859	С	VAL			44.571	28.334	14.719	1.00 17.53
ATOM	2860	0	VAL			43.678	27.764	14.021	1.00 17.13
MOTA	2861	CB	VAL	A	422	44.257	27.588	17.061	1.00 16.92
ATOM	2862		VAL			45.632	26.938	17.063	1.00 15.15
MOTA	2863	CG2	VAL			43.850	28.004	18.479	1.00 19.33
ATOM	2864	N	HIS	A	423	45.815	28.531	14.291	1.00 16.64
ATOM	2865	CA	HIS	A	423	46.264	28.112	12.940	1.00 16.92
MOTA	2866	C	HIS	А	423	47.792	28.038	12.906	1.00 17.46
MOTA	2867	0	HIS	А	423	48.461	28.105	13.981	1.00 17.20
MOTA	2868	CB	HIS	Α	423	45.755	29.111	11.889	1.00 15.85
ATOM	2869	CG	HIS	A	423	46.242	30.512	12.096	1.00 18.62
MOTA	2870	ND1	HIS	A	423	47.390	30.998	11.504	1.00 19.80
ATOM	2871	CD2	HIS	Α	423	45.758	31.522	12.857	1.00 17.42
ATOM	2872	CE1	HIS	A	423	47.590	32.245	11.892	1.00 18.22
ATOM	2873	NE2	HIS	A	423	46.615	32.586	12.714	1.00 18.53
ATOM	2874	N	ASP	Α	424	48.360	27.869	11.714	1.00 18.00
ATOM	2875	CA	ASP	Α	424	49.836	27.817	11.556	1.00 17.75
ATOM	2876	С	ASP	Α	424	50.194	28.804	10.453	1.00 18.36
MOTA	2877	0	ASP			49.294	29.527	9.935	1.00 20.02
ATOM	2878	CB	ASP			50.305	26.396	11.206	1.00 18.00
ATOM	2879	CG	ASP			49.545	25.791	10.037	1.00 19.08
ATOM	2880	OD1	ASP	Α	424	49.110	24.623	10.149	1.00 18.99
ATOM	2881	OD2				49.390	26.473	9.003	1.00 20.46
ATOM	2882	N	GLU			51.459	28.877	10.063	1.00 17.55
ATOM	2883	CA	GLU			51.813	29.853	9.015	1.00 18.77
ATOM	2884	C	GLU			51.497	29.379	7.601	1.00 16.95
ATOM	2885	ō	GLU			51.724	30.131	6.613	1.00 17.24
MOTA	2886	CB	GLU			53.289	30.239	9.112	1.00 18.65
ATOM	2887	CG	GLU			54.254	29.150	8.714	1.00 20.84
ATOM	2888	CD	GLU			55.632	29.697	8.381	1.00 21.89
MOTA	2889		GLU			56.481	28.901	7.936	1.00 22.61
ATOM	2890	OE2	GLU	A	425	55.867	30.920	8.559	1.00 22.65
MOTA	2891	N	PHE			50.955	28.171	7.476	1.00 14.60
ATOM	2892	CA	PHE			50.619	27.606	6.150	1.00 13.51
ATOM	2893	C	PHE			49.157	27.767	5.763	1.00 15.14
ATOM	2894	Ō	PHE			48.826	27.822	4.540	1.00 16.10
ATOM	2895	CB	PHE			51.001	26.127	6.109	1.00 14.53
MOTA	2896	CG	PHE			52.452	25.877	6.400	1.00 14.20
ATOM	2897		PHE			53.433	26.244	5.482	1.00 13.59
ATOM	2898		PHE			52.841	25.298	7.606	1.00 14.11
ATOM	2899		PHE			54.787	26.040	5.762	1.00 14.83
ATOM	2900		PHE			54.192	25.087	7.897	1.00 15.49
MOTA	2901	CZ	PHE			55.167	25.460	6.969	1.00 14.08
ATOM	2902	N	ARG			48.269	27.827	6.752	1.00 13.77
ATOM	2903	CA	ARG			46.824	27.985	6.469	1.00 14.89
MOTA	2904	C	ARG			46.130	28.695	7.615	1.00 15.43
ATOM	2905	0	ARG			46.630	28.710	8.781	1.00 14.58
ATOM	2906	CB	ARG			46.132	26.632	6.301	1.00 15.33
MOTA	2907	CG	ARG			46.959	25.518	5.707	1.00 16.84
ATOM	2908	CD	ARG			46.645	24.234	6.477	1.00 17.68
ATOM	2909	NE	ARG			45.994	23.230	5.655	1.00 16.69
MOTA	2910	CZ	ARG			45.701	21.998	6.062	1.00 15.45
MI ON	2710	L	DAA	n	30 I	10.701	22.990	0.002	2.03 20.20



ATOM	2911	NH1	ARG A 427		45.114	21.159	5.224	1.00 14.20
ATOM	2912	NH2	ARG A 427		45.981	21.603	7.296	1.00 13.31
ATOM	2913	N	THR A 428		44.976	29.269	7.317	1.00 15.28
ATOM	2914	CA	THR A 428		44.180	29.967	8.336	1.00 17.94
ATOM	2915	C	THR A 428		42.731	29.650	8.041	1.00 16.25
					42.400	29.165	6.923	1.00 14.77
MOTA	2916	0.	THR A 428					
ATOM	2917	CB	THR A 428		44.353	31.503	8.249	1.00 18.18
MOTA	2918		THR A 428		44.043	31.942	6.921	1.00 20.24
MOTA	2919		THR A 428		45.773	31.901	8.583	1.00 19.84
MOTA	2920	N	ALA A 429	•	41.860	29.901	9.009	1.00 16.14
ATOM	2921	CA	ALA A 429		40.423	29.677	8.803	1.00 16.03
ATOM	2922	С	ALA A 429		40.048	30.739	7.775	1.00 15.66
MOTA	2923	0	ALA A 429		40.808	31.738	7.574	1.00 14.51
ATOM	2924	CB	ALA A 429		39.656	29.898	10.105	1.00 17.08
ATOM	2925	N	ALA A 430		38.920	30.575	7.107	1.00 14.04
ATOM	2926	CA	ALA A 430		38.556	31.576	6.100	1.00 13.71
ATOM	2927	C.	ALA A 430		37.067	31.706	5.883	1.00 11.98
MOTA	2928	Ō	ALA A 430		36.271	30.754	6.166	1.00 12.33
ATOM	2929	СВ	ALA A 430		39.251	31.246	4.762	1.00 12.27
MOTA	2930	N-	VAL A 431		36.671	32.874	5.396	1.00 11.01
MOTA	2931	CA	VAL A 431		35.260	33.149	5.076	1.00 13.39
ATOM	2932	C	VAL A 431		35.344	33.773	3.697	1.00 15.69
ATOM	2933	0	VAL A 431		35.857	34.926	3.533	1.00 17.86
	2934	СВ	VAL A 431		34.624	34.145	6.056	1.00 17.50
MOTA						34.294	5.737	1.00 10.61
ATOM	2935		VAL A 431		33.148			
MOTA	2936		VAL A 431		34.818	33.659	7.494	
MOTA	2937	. N	GLU A 432		34.874	33.048	2.694	1.00 16.74
MOTA	2938	CA	GLU A 432		34.969	33.544	1.320	1.00 18.65
ATOM	2939	C	GLU A 432		33.681	33.414	0.530	1.00 18.40
MOTA	2940	0	GLU A 432	٠.	32.794	32.567	0.852	1.00.16.81
MOTA	2941	CB	GLU A 432		36.097	32.796	0.607	1.00 19.91
MOTA	2942	·CG	GLU A 432		37.460	33.031	1.241	1.00 24.66
MOTA	2943	CD	GLU A 432		38.466	31.930	0.935	1.00 27.80
MOTA	2944	OE1	GLU A 432		39.681	32.196	1.051	1.00 30.84
MOTA	2945	OE2	GLU A 432		38.049	30.799	0.595	1.00 28.87
MOTA	2946	N	GLY A 433		33.574	34.243	-0.504	1.00 18.95
MOTA	2947	CA	GLY A 433		32.408	34.244	-1.363	1.00 19.36
MOTA	2948	C	GLY A 433		32.504	35.385	-2.359	1.00 19.59
ATOM	2949	0	GLY A 433		33.489	36.173	-2.328	1.00 18.33
MOTA	2950	N	PRO A 434		31.511	35.539	-3.243	1.00 19.47
ATOM	2951	CA	PRO A 434		30.345	34.655	-3.285	1.00 19.72
ATOM	2952	С	PRO A 434		30.485	33.589	-4.353	1.00 19.98
ATOM	2953	0	PRO A 434		31.382	33.674		1.00 22.24
	2954	CB	PRO A 434		29.215	35.619		1.00 19.80
ATOM	2955	CG	PRO A 434		29.869	36.517	-4.616	1.00 19.70
ATOM	2956	CD	PRO A 434		31.261		-4.018	1.00 19.73
ATOM	2957	N	PHE A 435		29.624	32.583	-4.290	1.00 21.45
MOTA	2958	CA	PHE A 435		29.619	31.502	-5.292	1.00 22.31
MOTA	2959	C	PHE A 435		28.217	31.513	-5.872	1.00 24.39
ATOM	2960	o o	PHE A 435	-	27.207	31.636	-5.110	1.00 24.58
			PHE A 435		29.924		-4.636	1.00 22.02
ATOM	2961	CB				30.155		
ATOM	2962	CG	PHE A 435		31.215	30.141		1.00 20.80
MOTA	2963		PHE A 435		31.232	30.392	-2.507	1.00 20.70
ATOM	2964		PHE A 435		32.424	29.945	-4.542	1.00 21.70
MOTA	2965		PHE A 435		32.432	30.451	-1.809	
MOTA	2966		PHE A 435		33.634	30.003	-3.853	1.00 21.68
ATOM ·	2967	CZ	PHE A 435	•	33.637	30.259		1.00 21.51
MOTA	2968	N	VAL A 436		28.117	31.396	-7.192	1.00 27.02
MOTA	2969	CA	VAL A 436	•	26.802	31.438	-7.872	1.00 29.79
MOTA	2970	C	VAL A 436		26.526	30.219	-8.739	1.00 32.85
MOTA	2971	0	VAL A 436		25.434	30.120		1.00 33.81
MOTA	2972	СB	VAL A 436	•	26.702	32.677	-8.787	1.00 28.98

ATOM	2973	CG1	VAL A	436	26.999	33.944	-7.996	1.00 29.00
ATOM	2974		VAL A		27.678	32.537	-9.947	1.00 28.49
ATOM	2975	N	THR A		27.473	29.292	-8.795	1.00 36.05
ATOM	2976	CA	THR A		27.305	28.089	-9.638	1.00 39.30
		C	THR A		26.582	26.979	-8.870	1.00 41.99
MOTA	2977						-9.276	
MOTA	2978	0	THR A		26.604	25.775		1.00 41.77
MOTA	2979	CB	THR A		28.690	27.592	-10.123	1.00 39.02
MOTA	2980	OG1	THR A		28.552	26.981	-11.408	1.00 42.51
MOTA	2981	CG2	THR A		29.280	26.578	-9.156	1.00 38.10
MOTA	2982	N	LEU A	438	25.908	27.368	-7.794	1.00 45.33
MOTA	2983	CA	LEU A	438	25.199	26.417	-6.901	1.00 49.22
MOTA	2984	С	LEU A	438	23.753	26.016	-7.165	1.00 50.49
MOTA	2985	Ō	LEU A		22.869	26.878	-7.466	1.00 51.99
MOTA	2986	СВ	LEU A		25.276	26.944	-5.473	1.00 50.30
MOTA	2987	CG	LEU A		26.027	28.269	-5.358	1.00 50.73
	2988		LEU A		25.108	29.457	~5.584	1.00 50.27
MOTA					26.629	28.328	-4.001	1.00 51.67
ATOM	2989		LEU A				-7.037	1.00 52.67
ATOM	2990	N	ASP A		23.505	24.715		
MOTA	2991	CA	ASP A		22.149	24.128	-7.172	
MOTA	2992	С	ASP A		21.690	24.224	-5.722	1.00 56.96
MOTA	2993	0	ASP A		21.757	23.221	-4.945	1.00 57.33
MOTA	29 94	CB	ASP A	439	22.240	22.657	-7.586	1.00 56.39
MOTA	2995	CG	ASP A	439	20.879	21.993	-7.695	1.00 57.68
MOTA	2996	OD1	ASP A	439	20.046	22.178	-6.781	1.00 57.75
ATOM	2997		ASP A		20.645	21.274	-8.692	1.00 58.18
MOTA	2998	N	MET A		21.233	25.407	-5.337	1.00 58.71
ATOM	2999	CA	MET A		20.841	25.656	-3.944	1.00 60.87
ATOM	3000	C	MET A		19.435	26.215	-3.713	1.00 62.52
ATOM	3001	o	MET A		19.247	27.451	-3.489	1.00 63.93
	3001	CB	MET A		21.916	26.569	-3.346	1.00 60.48
MOTA		CG	MET A		21.523	27.456	-2.201	1.00 60.72
ATOM	3003				22.755	28.755	-2.086	1.00 59.28
ATOM	3004	SD	MET A				-3.543	1.00 59.46
MOTA	3005	CE	MET A		22.367	29.689		1.00 53.40
MOTA	3006	N	GLU A		18.435	25.343	-3.765	
MOTA	3007	CA	GLU A		17.042	25.774	-3.514	1.00 65.54
MOTA	3008	C	GLU A		16.356	24.847	-2.518	1.00 64.49
MOTA	3009	0	GLU A		15.998	25.285	-1.375	1.00 65.36
ATOM	3010	CB	GLU A		16.229	25.847	-4.815	1.00 67.99
MOTA	3011	CG	GLU A		16.500	24.745	-5.822	1.00 70.98
ATOM	3012	CD	GLU A	441	17.353	25.228	-6.981	1.00 72.23
ATOM	3013	OE1	GLU A	441	18.507	25.646	-6.742	1.00 73.24
ATOM	3014	OE2	GLU A	441	16.867	25.194	-8.132	1.00 73.30
ATOM	3015	N	ASP A	442	16.170	23.585	-2.896	1.00 61.29
ATOM	3016	CA	ASP A		15.519	22.616	-1.986	1.00 58.37
ATOM	3017	C	ASP A		16.504	21.966	-1.018	1.00 55.47
ATOM	3018	ō	ASP A		16.615	20.704		1.00 54.59
ATOM	3019	CB	ASP A		14.800	21.530		1.00 59.93
MOTA	3020	CG	ASP A		13.298	21.616		1.00 60.90
					12.689	22.478		1.00 61.34
ATOM	3021		ASP A		12.729	20.832		1.00 61.81
ATOM	3022		ASP A					1.00 51.31
MOTA	3023	N	CYS A		17.207	22.790		1.00 31.31
MOTA	3024	CA	CYS A		18.200	22.281		
ATOM	3025	C	CYS A		17.635	22.156		1.00 46.40
MOTA	3026	0	CYS A		18.168	21.373		1.00 44.04
ATOM .	3027	CB	CYS A	443	19.421	23.198		1.00 48.61
MOTA	3028	SG	CYS A	443	20.176	23.339		1.00 46.95
ATOM	3029	N	GLY A	444	16.566	22.895		1.00 45.40
ATOM	3030	CA	GLY F		15.953	22.846		1.00 45.06
ATOM	3031	C	GLY A		15.011	21.673	3.899	1.00 45.25
ATOM	3032	ō	GLY A		14.271	21.264		1.00 44.97
ATOM	3033	N		445	15.018	21.109		1.00 44.97
ATOM	3034	CA		445	14.140	19.968		1.00 44.48
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MOTA	3035	С	TYR A	445		12.778	20.467	5.882	1.00 45.23
	3036	o	TYR A			12.662	21.558	6.530	
ATOM			TYR A						
ATOM	3037	CB				14.801	19.172	6.531	1.00 43.11
MOTA	3038	CG	TYR A			13.918	17.997	6.871	1.00 42.75
_	. 3039	CD1				13.846	16.905	6.010	1.00 42.58
MOTA	3040	CD2	TYR A			13.170	17.998	8.049	1.00 42.27
MOTA	3041	CE1	TYR A	445		13.042	15.820	6.327	1.00 41.99
ATOM	3042	CE2	TYR A	445		12.358	16.917	8.360	1.00 43.20
ATOM	3043	CZ	TYR A	445		12.289	15.835	7.503	1.00 41.98
ATOM	3044	ОН	TYR A			11.490	14.751	7.810	1.00 20.00
ATOM	3045	N	ASN A			11.746	19.699	5.550	1.00 45.69
ATOM	3046	CA	ASN A			10.359	20.012	5.947	1.00 48.64
ATOM.	3047		ASN A			9.776	18.726	6.524	1.00 50.90
						9.894			
ATOM	3048	0	ASN A				17.625	5.896	1.00 51.59
ATOM	3049	CB	ASN A			9.537	20.470	4.738	1.00 48.19
ATOM	3050	CG	ASN A			9.975	21.827	4.213	1.00 48.18
ATOM	3051		ASN A			9.926	22.858	4.950	1.00 48.63
ATOM	3052	ND2				10.403	21.867	2.957	1.00 48.04
MOTA	3053	N	ILE A	447	•	9.165	18.826	7.700	1.00 53.94
ATOM	3054	CA	ILE A	447		8.569	17.650	8.388	1.00 55.99
ATOM	3055	C.	ILE A	447		7.720	16.772	7.463	1.00 57.01
ATOM	3056	o ·	ILE A	447	•	7.449	17.195	6.318	1.00 58.11
ATOM	3057	СВ	ILE A	447		7.699	18.105	9.577	1.00 55.86
MOTA		CG1	ILE A	447		8.488	19.086	10.450	1.00 56.28
ATOM	3059	CG2	ILE A			7.267	16.900	10.406	1.00 56.92
ATOM	3060	CD1	ILE A			9.759	18.505	11.037	1.00 55.79
MOTA	3061	OXT	ILE A			7.328	15.666	7895	1.00 57.55
	3062	N	SER P	1		35.528	15.672	28.238	1.00 37.53
ATOM									
MOTA	3063	CA	SER P	1		34.172	16.082	28.590	1.00 36.72
MOTA	3064	C.	SER P	.1		33.508	16.863	27.450	1.00 34.75
MOTA	3065	o	SER P	1		34.132	17.643	26.742	1.00 36.46
MOTA	3066	CB	SER P	1		34.248	16.949	29.848	1.00 37.77
ATOM	3067	OG	SER P	1		33.152	17.865	29.853	1.00 40.82
MOTA	3068	N	GLU P	2		32.203	16.601	27.257	1.00 32.86
ATOM	3069	CA	GLU P	2		31.513	17.216	26.129	1.00 32.80
ATOM	3070	С	GLU P	2		30.218	17.906	26.552	1.00 31.23
MOTA	3071	0 .	GLU P	. 2		29.435	17.401	27.348	1.00 31.31
ATOM	3072	CB	GLU P	. 2		31.275.	16.167	25.027	1.00 33.64
ATOM	3073	CG	GLU P	. 2		31.096	17.096	23.826	1.00 37.41
ATOM	3074	CD	GLU P	2		31.076	15.940	22.852	1.00 38.37
ATOM	3075	OE1		. 2		31.996	15.134	22.983	1.00 39.04
ATOM	3076	ÖE2	GLU P	. 2		30.175	15.798	22.037	1.00 39.43
		- ·-		_					
ATOM	3077 3.078	N	VAL P	3		29.742	19.344	26.106	1.00 27.98
ATOM		CA	VAL P	. 3		28.367	19.820	26.101	1.00 26.44
MOTA	3079	Ċ	VAL P	3		27.717	19.598	24.735	1.00 26.26
MOTA	3080	0	VÁL P	3		28.371	19.580	23.701	1.00 25.48
MOTA	3081	CB	VAL P	3		28.377	21.311	26.429	1.00 25.89
ATOM	3082		VAL P	3		28.684	21.516	27.911	1.00 27.07
MOTA	3083	CG2	VAL P	. 3		29.431	22.012	25.594	1.00 23.97
MOTA .	3084	N	ASN P	. 4	-	26.361	19.591	25.174	1.00 25.89
ATOM	3085	CA	ASN P	4		25.421	19.254	24.075	1.00 26.64
ATOM	3086	C	ASN P	. 4		24.027	19.825	24.452	1.00 26.87
MOTA	3087	0	ASN P	4		23.116	19.163	25.077	1.00 27.10
ATOM	3088	СВ	ASN P	4		25.349	17.766	23.876	1.00 27.95
ATOM	3089	CG	ASN P	4		26.498	17.245	22.971	1.00 29.39
MOTA	3090		ASN P	4	*	26.499	17.409	21.723	1.00 23.35
	3090		ASN P	. 4					1.00 31.90
ATOM						27.489	16.617	23.603	
ATOM	3092	N	STA P	5		24.115	21.101	24.323	1.00 25.26
MOTA	3093	CA	STA P	5		22.965	21.865	24.929	1.00 25.83
MOTA	3094	CB .		. 5.		23.683	22.681	26.021	1.00 27.28
MOTA	3095	CG	STA P	. 5		24.378	22.057	27.197	1.00 28.07
MOTA	3096	CD1	STA P	, 5		25.002	23.077	28.182	1.00 27.46



MOTA	3097	CD2	STA	Р	5	23.280	21.130	27.828	1.00 25.47
MOTA	3098	CH	STA	Ρ	5	22.223	22.851	23.940	1.00 25.86
ATOM	3099	OH	STA	Ρ	5	23.028	23.679	23.298	1.00 25.23
ATOM	3100	CM	STA	P	5	21.372	21.980	23.048	1.00 27.11
ATOM	3101	С	STA		5	20.420	21.340	24.125	1.00 27.81
ATOM	3102	ō	STA		5	20.241	20.065	24.095	1.00 25.70
ATOM	3103	N	VAL		6	19.339	22.479	23.764	1.00 26.04
ATOM	3104	CA	VAL		6	18.037	21.953	24.156	1.00 27.12
ATOM	3105	C	VAL		6	17.496	20.965	23.121	1.00 27.36
						17.795	20.903	21.936	1.00 27.30
ATOM	3106	0	VAL	P	6				1.00 20.37
ATOM	3107	CB		P	6	17.073	23.130	24.312	
ATOM	3108		VAL		6	16.433	23.463	22.965	1.00 26.70
MOTA	3109		VAL		6	15.985	22.781	25.311	1.00 28.74
MOTA	3110	N	ALA		7	16.702	19.998	23.617	1.00 28.68
MOTA	3111	CA	ALA		7	16.158	18.986	22.720	1.00 32.14
ATOM	3112	С	ALA		7	14.774	19.377	22.197	1.00 32.99
MOTA	3113	0	ALA		7	14.040	20.149	22.801	1.00 32.08
ATOM	3114	СВ	ALA		7	16.072	17.666	23.489	1.00 31.38
MOTA	3115	N	GLU		8	14.443	18.843	21.007	1.00 36.10
MOTA	3116	CA	GLU	P	8	13.144	19.143	20.418	1.00 39.90
MOTA	3117	С	GLU	Р	8	12.012	18.425	21.158	1.00 41.72
MOTA	3118	0	GLU	P	8	12.189	17.359	21.733	1.00 41.52
MOTA	3119	CB	GLU	Ρ	8	13.172	18.705	18.952	1.00 39.88
MOTA	3120	CG	GLU	P	8	14:037	19.626	18.090	1.00 41.02
MOTA	3121	CD	GLU	P	8	13.896	19.235	16.637	1.00 41.83
ATOM	3122	0E1	GLU	P	8	14.911	19.052	15.979	1.00 41.60
ATOM	3123	OE2	GLU	Ρ	8	12.765	19.124	16.169	1.00 41.88
ATOM	3124	N	PHE	Ρ	9	10.811	18.986	21.162	1.00 45.62
MOTA	3125	CA	PHE	P	9	9.677	18.356	21.865	1.00 49.63
ATOM	3126	С	PHE	P	9	9.382	16.960	21.337	1.00 50.61
ATOM	3127	Ō	PHE	P	9	9.156	16.839	20.116	1.00 51.38
ATOM	3128	CB	PHE	P	9	8.451	19.245	21.670	1.00 50.65
ATOM	3129	CG	PHE	P	9	8.607	20.501	22.499	1.00 52.48
MOTA	3130	CD1		P	9	8.278	20.493	23.849	1.00 52.80
ATOM	3131	CD2	PHE		9	9.073	21.659	21.899	1.00 53.12
MOTA	3132	CEl			9	8.420	21.651	24.600	1.00 53.74
ATOM	3133	CE2	PHE		9	9.215	22.817	22.659	1.00 53.61
ATOM	3134	CZ	PHE		9	8.890	22.817	24.010	1.00 54.24
ATOM	31:35	OXT	PHE		9	9.383	16.011	22,152	1.00 51.56
ATOM	3136	OH2	TIP		2	37.673	4.149	14.933	1.00 18.73
ATOM	3137	OH2	TIP		3	37.999	19.019	28.545	1.00 20.36
ATOM	3138	OH2	TIP		12	46.550	23.555	9.446	1.00 16.05
ATOM	3139		TIP		14	18.354	26.505	28.719	1.00 14.14
ATOM	3140		TIP		15	33.073	10.884	15.835	1.00 14.30
ATOM	3141		TIP		16	15.032	34.698	31.070	1.00 11.96
ATOM	3142		TIP		17	7.170	35.908	33.277	1.00 16.70
ATOM	3143		TIP		19	16.624	32.704	28.166	1.00 15.10
			TIP		20	35.078	42.552	29.609	1.00 19.72
ATOM	3144				21	40.457	30.360	27.755	1.00 16.31
ATOM	3145	OH2				52.263	20.430	9.725	1.00 20.11
ATOM	3146	OH2			22	20.720		14.822	1.00 20.11
ATOM	3147		TIP		23		20.412		1.00 12.00
MOTA	3148		TIP		24	33.413	15.317	~5.393	
ATOM	3149	OH2			25	38.275	25.072	23.469	1.00 13.40 1.00 19.86
ATOM	3150	OH2			27	16.591	21.729	7.186	1.00 19.88
ATOM	3151	OH2			28	21.798	19.346	19.780	
ATOM	3152	OH2			29	17.533	34.724	25.177	1.00 16.69
MOTA	3153	OH2			30	29.162	27.768	25.821	1.00 19.19
MOTA	3154	OH2			31	40.631	28.021	16.946	1.00 14.53
MOTA	3155	OH2			32	32.428	32.415	17.998	1.00 10.42
MOTA	3156		TIP		33	11.884	34.798	21.161	1.00 23.00
ATOM	3157	OH2			34	27.837	25.769	-5.173	1.00 33.18
MOTA	3158	OH2	TIP	С	35	12.372	31.279	28.339	1.00 16.96



39.263 28.648 25.755 1.00 9.84 36 MOTA 3159 OH2 TIP C 38.924 30.840 30.171 1.00 13.35 OH2 TIP C 3160 40 MOTA 18.085 18.989 18.858 1.00 16.60 3161 OH2 TIP C 41 MOTA 7..300 35.692 30.168 1.00 19.22 . 3162 OH2 TIP C 42 MOTA 43 14.250 32.017 30.405 1.00 18.32 OH2 TIP C ATOM * 3163 37.440 22.761 1.00 23.96 1.333 MOTA 3164 OH2 TIP C 44 29.932 39.949 32.969 1.00 22.64 45 MOTA 3165 OH2 TIP C 29.433 17.902 20.935 1.00 16.15 OH2 TIP C 46 29.433 17.902 20.935
OH2 TIP C 47 53.536 22.468 21.774
OH2 TIP C 48 40.180 15.699 -0.272
OH2 TIP C 49 14.955 25.973 25.745
OH2 TIP C 50 38.595 6.527 3.885
OH2 TIP C 51 48.551 24.793 17.574
OH2 TIP C 52 20.747 27.407 17.869
OH2 TIP C 53 26.489 18.730 30.746
OH2 TIP C 54 38.723 11.162 19.249
OH2 TIP C 55 33.881 26.191 31.382
OH2 TIP C 56 13.322 31.213 40.027
OH2 TIP C 57 19.497 16.134 41.439
OH2 TIP C 58 38.469 37.062 5.695 46 MOTA 3166 OH2 TIP C 1.00 21.62 3167 MOTA 1.00 12.15 ATOM 3168 1.00 11.98 3169 ATOM 1.00 23.66 ATOM 3170 1.00 18.30 MOTA 3171 1.00 8.25 MOTA 3172 1.00 26.59 3173 ATOM 1.00 11.49 3174 \mathtt{MOTA} 1.00 19.21 MOTA 3175 1.00 15.61 ATOM 3176 1.00 26.82 3177 MOTA 38.469 37.062 5.695 1.00 23.10 58 3178 OH2 TIP C ATOM 15.894 3.122 1.00 18.45 59 45.575 MOTA 3179 OH2 TIP C 39.615 25.333 -1.743 1.00 20.09 60 MOTA .3180 OH2 TIP C 32.158 37.928 32.431 1.00 12.17 MOTA 3181 OH2 TIP C 61 46.793 19.609 24.847 37.031 45.957 19 717 46.793 19.609 22.823 1.00 19.81 OH2 TIP C 62 ATOM 3182 -0.659 1.00 29.98 MOTA OH2 TIP C 63 3183 3.836 1.00 18.88 OH2 TIP C 64 MOTA 3184 36.189 33.100 17.653 1.00 10.63 OH2 TIP C 65 ATOM 3185 31.177 25.020 24.150 1.00 28.40 66 MOTA 3186 OH2 TIP C 46.181 23.210 18.466 1.00 20.41 21.756 10.923 7.943 1.00 22.80 67 OH2 TIP C MOTA 3187 68 69 3188 OH2 TIP C ATOM 12.936 36.695 30.481 1.00 17.63 33.713 44.843 8.382 1.00 30.49 21.051 41.550 39.982 1.00 31.15 OH2 TIP C MOTA 3189 OH2 TIP C 70 ATOM 3190 MOTA 3191 OH2 TIP C 71 26.815 38.732 3.198 1.00 22.61 41.656 24.820 21.177 1.00 19.69 ATOM . OH2 TIP C 72 3192 25.521 30.139 47.617 1.00 19.69 25.497 46.537 15.336 1.00 29.67 ATOM 3193 OH2 TIP C 73 74 ATOM 3194 OH2 TIP C 75 OH2 TIP C MOTA 3195 7.708 28.422 41.027 1.00 26.00 76 OH2 TIP C MOTA 3196 25.650 18.585 27.821 1.00 17.30 77 MOTA 3197 OH2 TIP C 35.124 16.582 21.374 1.00 15.44 16.806 29.258 45.952 1.00 22.64 3198 OH2 TIP C 78 MOTA 79 OH2 TIP C ATOM 3199 29.365 80 7.305 14.767 1.00 28.00 3200 OH2 TIP C ATOM 36.259 9.577 -0.018 1.00 36.72 81 3201 OH2 TIP C MOTA 82 5.598 37.375 35.367 1.00 29.64 MOTA 3202 OH2 TIP C 14.256 22.267 9.863 1.00 20.30 34.533 14.826 41.318 1.00 35.70 83 3203 OH2 TIP C MOTA 84 3204 OH2 TIP C ATOM 14.253 38.931 17.469 1.00 22.15 40.762 43.633 8.075 1.00 32.27 85 3205 OH2 TIP C ATOM ATOM . 3206 OH2 TIP C 86 20.139 38.471 47.202 1.00 19.79 3207 OH2 TIP C 87 MOTA 49.003 25.388 48.376 21.580 14.809 1.00 16.95 MOTA 3208 OH2 TIP C 88 21.346 1.00 26.51 3209 OH2 TIP C 89 ATOM 38.281 15.314 27.561 1.00 34.16 OH2 TIP C 90 MOTA 3210 8.631 39.984 34.095 1.00 41.37 OH2 TIP C 91 MOTA 3211 50.906 23.612 53.785 20.060 24.823 42.619 20.744 1.00 52.18 OH2 TIP C 92 ATOM 3212 24.538 1.00 24.16 MOTA 3213 OH2 TIP C 93 -1.00 21.18 11:579 ATOM 3214 OH2 TIP C 94 25.075 40.830 43.416 13.417 33.278 1.00 38.65 45.083 6.146 3215 OH2 TIP C 95 ATOM . 25.584 1.00 18.31 3216 18.443 OH2 TIP C 96 MOTA OH2 TIP C 97 43.416 22.239 18.182 1.00 19.16 3217 ATOM 1.00 31.15 3218 OH2 TIP C 98 34.174 40.223 ATOM 35.258 1.00 19.39 OH2 TIP C 99 3219 33.278 34.940 MOTA 16.214 16.638 1.00 44.74 11.125 ATOM 3220 OH2 TIP C 100

ATOM	3221	OH2 TIP	C 101	53.364	20.723	14.579	1.00 34.15
ATOM	3222	OH2 TIP		49.883	22.898	7.975	1.00 17.76
ATOM	3223		C 103	23.025	15.361	39.364	1.00 32.71
	_			9.989	41.920	29.368	
MOTA	3224						1.00 18.54
MOTA	3225	OH2 TIP		40.434	26.276	24.857	1.00 17.36
MOTA	3226	OH2 TIP		20.997	29.964	6.095	1.00 20.90
MOTA	3227	OH2 TIP	C 107	27.762	47.336	16.035	1.00 24.48
MOTA	3228	OH2 TIP	C 108	49.284	22.771	5.126	1.00 18.73
ATOM	3229	OH2 TIP	C 109	48.838	23.239	29.592	1.00 33.97
ATOM	3230	OH2 TIP		28.582	23.099	35.349	1.00 20.25
ATOM	3231	OH2 TIP		32.528	35.162	39.110	1.00 29.39
ATOM	3232		C 112	41.404	21.066	27.696	1.00 29.24
				41.566	30.795	24.916	1.00 29.24
ATOM	3233		C 113				
ATOM	3234	OH2 TIP		38.888	34.349	4.634	1.00 19.24
ATOM	3235		C 115	21.524	13.318	6.181	1.00 21.83
ATOM	3236		C 116	20.262	44.365	41.166	1.00 51.68
ATOM	3237	OH2 TIP	C 117	40.866	37.586	7.262	1.00 26.48
ATOM	3238	OH2 TIP	C 118	24.269	19.013	20.381	1.00 20.56
ATOM	3239	OH2 TIP	C 119	14.796	40.366	21.026	1.00 26.21
MOTA	3240	OH2 TIP	C 120	40.271	21.968	24.452	1.00 22.99
ATOM	3241	OH2 TIP	C 121	27.256	8.206	3.568	1.00 32.16
ATOM	.3242	OH2 TIP		38.453	23.426	21.155	1.00 20.65
ATOM	3243	OH2 TIP		39.489	30.192	18.787	1.00 19.64
MOTA	3244	OH2 TIP		49.479	24.877	3.120	1.00 15.38
				23.534	17.922	36.838	1.00 21.55
MOTA	3245	OH2 TIP					
MOTA	3246	OH2 TIP		24.481	13.568	37.531	1.00 33.00
ATOM	3247	OH2 TIP		27.515	37.075	45.132	1.00 32.65
ATOM	3248	OH2 TIP		20.903	11.530	10.774	1.00 25.13
ATOM	3249	OH2 TIP		16.996	37.117	6.834	1.00 26.72
ATOM	3250	OH2 TIP	C 130	42.280	39.848	5.806	1.00 39.08
MOTA	3251	OH2 TIP	C 131	15.426	37.238	14.643	1.00 27.36
ATOM	3252	OH2 TIP	C 132	47.740	29.973	16.321	1.00 27.58
ATOM	3253	OH2 TIP		52.162	19.864	18.278	1.00 19.10
ATOM	3254	OH2 TIP		47.805	11.416	4.529	1.00 30.40
ATOM	3255	OH2 TIP		20.920	22.905	41.964	1.00 23.80
ATOM	3256	OH2 TIP		27.784	19.013	-1.506	1.00 28.71
ATOM	3257	OH2 TIP		25.506	36.437	2.115	1.00 19.53
		OH2 TIP		6.347	36.058	44.801	1.00 30.54
MOTA	3258	_					
MOTA	3259	OH2 TIP		18.428	23.862	8.397	1.00 19.65
MOTA	3260	OH2 TIP		56.631	14.945	24.048	1.00 29.26
MOTA	3261	OH2 TIP		36.045	33.381	-3.424	1.00 39.63
MOTA	3262		C 142		14.180		1.00 31.49
MOTA	3263	OH2 TIP		8.614	22.301	31.526	1.00 30.94
MOTA	3264	OH2 TIP	C 144		38.736	31.440	1.00 44.64
ATOM	3265	OH2 TIP	C 145	21.002	20.115	40.621	1.00 23.34
MOTA	3266	OH2 TIP	C 146	36.343	37.533	7.628	1.00 25.43
ATOM	3267	OH2 TIP	C 147	13.944	44.970	51.125	1.00 40.01
MOTA	3268	OH2 TIP	C 148	12.509	22.964	23.735	1.00 33.44
MOTA	3269	OH2 TIP			6.398	6.686	1.00 30.50
ATOM	3270	OH2 TIP			30.018	41.695	1.00 29.12
	3271				19.454	17.419	1.00 26.72
ATOM		OH2 TIP		37.729	21.375	25.750	1.00 20.72
MOTA	3272	OH2 TIP					
ATOM	3273	OH2 TIP		36.922	28.170	33.507	1.00 42.28
ATOM	3274	OH2 TIP			29.766	32.277	1.00 19.72
ATOM	3275	OH2 TIP			19.732	11.775	1.00 37.67
MOTA	3276	OH2 TIP			28.327	48.310	1.00 40.64
ATOM	3277	OH2 TIP			46.759	12.106	1.00 40.48
MOTA	3278	OH2 TIP	C 158	22.361	9.339	13.691	1.00 44.57
ATOM	3279	OH2 TIP	C 159	26.097	16.601	36.996	1.00 27.61
ATOM	3280	OH2 TIP			24.669	14.501	1.00 39.22
ATOM	3281	OH2 TIP			33.316	38.299	1.00 37.21
ATOM	3282	OH2 TIP			43.316	6.583	1.00 32.14
			. –		_	·	



MOTA	3283	OH2 TIP	C -163		44.434	22.056	2.693	1.00 44.76
ATOM	3284	OH2 TIP	C 164	•	24.074	33.090	45.770	1.00 26.95
ATOM	3285		C 165		12.289	35.656	48.500	1.00 33.30
	-							
ATOM .	3286	OH2 TIP		•	19.499	27.253	51.538	1.00 48.93
ATOM:	3287	OH2 TIP	C 167	,1	28.896	14.390	20.410	1.00 32.12
MOTA	3288	OH2 TIP	C 168		7.799	34.543	25.107	1.00 34.11
	3289	OH2 TIP			41.359	33.697	5.939	1.00 29.72
ATOM								the state of the s
ATOM	3290	OH2 TIP			26.378	23.008	46.449	1.00 37.54
ATOM	3291	OH2 TIP	C 171		10.530	41.770	49.010	1.00 34.66
ATOM	3292	OH2 TIP	C 172		41.154	5.586	4.533	1.00 25.18
ATOM	3293	OH2 TIP			17.462	11.487	4.521	1.00 46.32
					7.600	39.527	37.113	1.00 36.37
ATOM	3294	OH2 TIP						
MOTA	3295	OH2 TIP			3.552	23.235	37.583	1.00 39.37
ATOM	3296	OH2 TIP	C 176		32.818	21.891	40.191	1.00 36.81
MOTA	3297	OH2 TIP	C 177		30.404	26.159	40.588	1.00 38.22
MOTA	3298	OH2 TIP			16.691	29.183		1.00 39.76
MOTA	3299	OH2 TIP			16.247	47.986	22.417	1.00 32.19
MOTA	3300	OH2 TIP			37.394	44.558	11.594	1.00 39.03
MOTA	3301	OH2 TIP	C 181		53.552	27.209	11.822	1.00 47.97
MOTA	3302	OH2 TIP	C 182		10.503	32.709	12.025	1.00 38.41
ATOM	3303	OH2 TIP	C 183		17.985	14.916	28.259	1.00 36.86
MOTA	3304	OH2 TIP			25.047		12.174	1.00 49.92
								1.00 40.29
MOTA	3305	OH2 TIP			16.402	15.741	36.532	
MOTA	3306	OH2 TIP			51.364	22.471	17.335	1.00 28.11
MOTA	3307	OH2 TIP	C 187		25.633	28.369	50.282	1.00 42.57
ATOM	3308	OH2 TIP	C 188		35.183	14.816	0.037	1.00 36.60
ATOM	3309	OH2 TIP	C 189		8.318	26.536	23.386	1.00 44.75
ATOM	3310	OH2 TIP			47.893	17.794	24.745	1.00 42.51
MOTA	3311	OH2 TIP			2.728	32.293	36.650	1.00 38.36
ATOM	3312	OH2 TIP	C 192		30.315	9.929	15.860	1.00 39.58
ATOM -	3313	OH2 TIP	C 193		29.613	40.378	2.225	1.00 41.26
ATOM	3314		C 194		14.241	43.934	16.316	1.00 43.60
ATOM	3315	OH2 TIP			48.673	31.215	7.801	1.00 32.67
MOTA	3316	OH2 TIP			10.948	21.963	18.969	1.00 41.87
MOTA	3317	OH2 TIP	C 197		37.378	39.077	3.714	1.00 35.77
MOTA	3318	OH2 TIP	C 198		24.488	11.993	21.654	1.00 38.05
ATOM	3319	OH2 TIP	C 199		47.986	31.378	4.946	1.00 48.02
ATOM	3320	OH2 TIP			15.373	46.520	15.659	1.00 45.30
MOTA					29.464	40.417	40.154	1.00 40.62
	3321							
MOTA	3322	OH2 TIP			56.018	18.652	7.189	1.00 43.28
MOTA	3323	OH2 TIP	C 203		36.508	17.526	41.765	1.00 61.21
MOTA	3324	OH2 TIP	C 204		36.132	36.523	-0.637	1.00 43.56
MOTA	3325	OH2 TIP	C 205		9.832	29.974	46.230	1.00 47.33
ATOM	3326		C 206		12.086	37.731	18.949	1.00 44.12
								1.00 40.03
ATOM	3327		C 207		4.729	26.744	22.711	
MOTA	3328		C 208		9.555	36.540	23.357	1.00 46.94
MOTA	3329	OH2 TIP	C 209		23.046	47.732	4.343	1.00 48.13
MOTA	3330	OH2 TIP	C 210		39.932	44.592	5.460	1.00 64.51
MOTA	3331		C 211		17.996	41.071	6.267	1.00 48.35
		OH2 TIP				46.493	17.139	1.00 39.09
ATOM	3332				17.866			
MOTA	3333	OH2 TIP			55.520	11.908	17.658	1.00 43.06
MOTA	3334	OH2 TIP			3.059	35.093	42.826	1.00 38.97
MOTA	3335	OH2 TIP	C 215		31.593	14.910	43.677	1.00 44.01
MOTA	3336	OH2 TIP		,	33.045	23.673	44.607	1.00 45.50
ATOM	3337	OH2 TIP			42.870	35.555		1.00 29.79
								1.00 56.65
MOTA	3338	OH2 TIP			4.112	25.648	42.564	•
MOTA	3339	OH2 TIP			48.260	8.547	20.446	1.00 47.85
ATOM .	.3340	OH2 TIP	C 220		-0.925	31.171	41.173	1.00 36.99
MOTA	3341		C 221		41.791	22.878	0.132	1.00 56.14
ATOM	3342		C 222		7.088	25.685	41.540	1.00 47.43
	3343	OH2 TIP			24.815	4.785	13.582	1.00 47.96
ATOM							15.174	1.00 48.76
MOTA	3344	OH2 TIP	C 224		40.690	4.520	T 7 . T / 4	7.00 40.70.

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MOTA	3345	OH2 TIP C 225	10.029	32.425	18.562	1.00 36.30
MOTA	3346	OH2 TIP C 226	22.346	37.737	48.941	1.00 34.15
ATOM	3347	OH2 TIP C 227	16.274	17.012	19.693	1.00 27.63
ATOM	3348	OH2 TIP C 228	35.332	13.692	20.375	1.00 37.59
ATOM	3349	OH2 TIP C 229	41.228	36.673	22.908	1.00 57.59
ATOM	3350	OH2 TIP C 230	17.416	42.030	50.226	1.00 31.38
MOTA	3351	OH2 TIP C 230	18.428	39.213		
			· ·		52.835	1.00 40.43
ATOM	3352	OH2 TIP C 232	42.243	43.386	25.548	1.00 48.60
MOTA	3353	OH2 TIP C 233	14.081	18.701	0.364	1.00 32.87
ATOM	3354	OH2 TIP C 234	41.421	41.332	28.531	1.00 54.67
MOTA	3355	OH2 TIP C 235	42.772	36.396	11.892	1.00 41.24
ATOM	3356	OH2 TIP C 236	13.068	13.733	28.653	1.00 42.66
·MOTA	3357 ·		10.850	26.738	7.811	1.00 40.46
MOTA	3358	OH2 TIP C 238	16.253	20.926	45.776	1.00 44.60
MOTA	3359	OH2 TIP C 239	32.681	31.139	43.220	1.00 42.20
MOTA	3360	OH2 TIP C 240	56.267	22.254	9.280	
ATOM	3361	OH2 TIP C 241	12.553	25.304	9.942	1.00 38.77
ATOM	3362	OH2 TIP C 242	50.727	9.516	16.775	1.00 33.38
MOTA	3363	OH2 TIP C 243	31.871	41.347	0.512	1.00 47.78
MOTA	3364	OH2 TIP C 244	10.008	45.092	37.807	1.00 39.52
MOTA	3365	OH2 TIP C 245	14.551	39.030	6.708	1.00 44.26
MOTA	3366	OH2 TIP C 246	26.955	18.903	-5.135	1.00 42.54
MOTA	3367	OH2 TIP C 247	39.916	22.478	18.854	1.00 33.22
MOTA	3368	OH2 TIP C 248	40.431	40.824	22.426	1.00 35.58
ATOM	3369	OH2 TIP C 249	52.081	23.408	10.759	1.00 42.53
MOTA	3370	OH2 TIP C 250	12.078	16.710	24.149	1.00 32.37
MOTA	3371	OH2 TIP C 251	54.111	15.908	8.256	1.00 44.58
ATOM	3372	OH2 TIP C 252	33.950	12.827	-1.753	1.00 27.02
MOTA	3373	OH2 TIP C 253	-0.775	26.703	40.353	1.00 43.64
ATOM	3374	OH2 TIP C 254	1.937	33.711	40.561	1.00 42.67
ATOM	3375	OH2 TIP C 255	8.008	24.066	18.824	1.00 51.45
MOTA	3376	OH2 TIP C 256	11.765	27.465	3.635	1.00 47.34
ATOM	3377	OH2 TIP C 257	27.863	43.878	9.233	1.00 32.44
MOTA	3378	OH2 TIP C 258	18.655	30.114	4.303	1.00 33.13
MOTA	3379	OH2 TIP C 259	21.592	19.085	-3.960	1.00 39.86
MOTA	3380	OH2 TIP C 260	41.876	24.067	25.906	1.00 26.34
MOTA	3381	OH2 TIP C 261	46.651	10.240	2.171	1.00 44.38
MOTA	3382	OH2 TIP C 262	32.536	15.827	32.477	1.00 43.28
ATOM	3383	OH2 TIP C 263	12.479	39.205	50.359	1.00 47.33
ATOM	3384	OH2 TIP C 264	0.850	27.980	38.316	1.00 43.45
MOTA	3385	OH2 TIP C 265	49.605	7.356	18.061	1.00 66.01
ATOM	3386	OH2 TIP C 266	30.177	40.365	-3.235	1.00 44.45
ATOM	3387	OH2 TIP C 267	39.818	12.364	0.512	1.00 48.84
ATOM	3388	OH2 TIP C 268	38.149	44.716	27.884	1.00 51.18
ATOM	3389	OH2 TIP C 269	37.156	37.062	30.528	1.00 35.17
ATOM	3390	OH2 TIP C 270	51.808	7.097	12.435	1.00 51.69
ATOM	3391	OH2 TIP C 271	54.351	12.626	12.471	1.00 47.45
MOTA	3392	OH2 TIP C 272	50.835	31.155	13.092	1.00 55.05
ATOM	3393	OH2 TIP C 273	12.159	35.313	52.133	1.00 52.38
ATOM	3394	OH2 TIP C 274	21.002	44.489	13.037	1.00 39.70
ATOM	3395	OH2 TIP C 275	37.936	23.627	34.221	1.00 48.56
ATOM	3396	OH2 TIP C 276	45.844	30.935	31.365	1.00 43.24
ATOM	3397	OH2 TIP C 277	38.831	48.015	15.554	1.00 49.83
ATOM	3398	OH2 TIP C 278	5.630	28.150	44.576	1.00 48.10
ATOM	3399	OH2 TIP C 279	8.600	24.000	45.727	1.00 49.27
ATOM	3400	OH2 TIP C 280	54.276	20.854	7.807	1.00 45.27
ATOM	3400	OH2 TIP C 280	3.544	34.696	46.365	1.00 43.63
ATOM	3401	OH2 TIP C 281	24.214			1.00 48.04
ATOM	3402	OH2 TIP C 282	7.099	46.264	46.163	1.00 48.04
	3403	OH2 TIP C 283	36.469	32.072	19.549	1.00 54.97
MOTA MOTA	3404	OH2 TIP C 284 OH2 TIP C 285	34.660	22.374 13.757	41.355 23.756	1.00 45.46
ATOM	3405	OH2 TIP C 285	28.516	42.981	5.402	1.00 43.40
ATOM	2400	ONZ TIF C 200	20.310	46.30T	5.404	1.00 33.30



ATOM	3407	OH2 TIP C	287	35.579	4.929	12.012	1.00 52.07
ATOM	3408		288	22.974	49.682	24.299	1.00 53.67
			289	3.725	31.464	46.354	1.00 46.43
ATOM	3409						
ATOM	3410	OH2 TIP C		27.340	39.594	-2.191	1.00 56.89
MOTA	3411	OH2 TIP C		33.413	34.856	32.335	1.00 31.78
MOTA	3412		292	43.340	7.715	8.063	1.00 43.53
ATOM	3413	OH2 TIP C	293	28.243	21.392	-4.937	1.00.38.33
ATOM	3414	OH2 TIP C	294	49.389	26.590	35.796	1.00 45.66
ATOM	3415	OH2 TIP C		28.948	15.824	33.796	1.00 52.48
ATOM	3416	OH2 TIP C		27.347	13.383	37.207	1.00 48.27
ATOM	3417	OH2 TIP C	297	38.485	26.090	36.901	1.00 48.92
			298	12.120	20.265	11.506	1.00 50.10
ATOM	3418			36.480	36.306	38.613	1.00 50.38
ATOM	3419	OH2 TIP C					1.00 38.37
ATOM	3420	OH2 TIP C		31.471	16.463	35.507	
MOTA	3421		301	42.889	5.274	2.358	1.00 33.49
ATOM	3422		302	23.548	44.173	32.246	1.00 39.09
MOTA	3423		303	13.465	43.978	13.054	1.00 52.67
ATOM	3424		304	25.133	43.053	4.111	1.00 52.03
ATOM	3425	OH2 TIP C	305	33.587	24.652	39.392	1.00 49.48
ATOM .	3426	OH2 TIP C	306	39.063	28.353	1.979	1.00 47.89
MOTA	3427	OH2 TIP C	307	49.357	35.834	12.150	1.00 49.22
ATOM	3428	OH2 TIP C	308	27.159	46.386	33.347	1.00 49.50
ATOM	3429	OH2 TIP C	309	9.510	21.769	39.704	1.00 47.95
ATOM	3430		310	34.885	32.959	39.205	1.00 51.26
ATOM	3431		311	30.980	6.002	9.747	1.00 56.02 -
ATOM	3432	OH2 TIP C		43.802	34.511	14.853	1.00 41.89
ATOM	3433	OH2 TIP C	313	36.834	4.382	5.254	1.00 39.04
ATOM	3434		314	12.453	30.429	47.461	1.00 47.60
	3435		315	39.685	40.144	30.944	1.00 54.68
MOTA			316	45.982	20.840	31.078	1.00 47.99
MOTA	3436		317	32.815	36.023	42.050	1.00 47.07
ATOM	3437						
ATOM	3438	OH2 TIP C	318	17.877	37.802	-3.699	1.00 56.30
ATOM	3439	•	319	53.681	9.633	16.525	1.00 55.34
MOTA	3440		320	21.577	43.070	52.229	1.00 49.54
MOTA	3441	OH2 TIP C	321	6.139	45.122	36.565	1.00 44.40
ATOM	3442	OH2 TIP C	322	34.695	13.561	26.782	1.00 45.99
MOTA	3443	OH2 TIP C	323	17.990	33.946	-9.976	1.00 56.88
ATOM	3444	OH2 TIP C	324	25.587	50.416	28.268	1.00 52.75
ATOM	3445	OH2 TIP C	325	27.744	42.608	42.266	1.00 44.66
MOTA	3446	OH2 TIP C	326	48.357	32.815	33.851	1.00 57.98
ATOM	3447	OH2 TIP C		61.047	18.004	17.692	1.00 51.30
ATOM	3448			17.327	11.069	11.972	1.00 48.28
ATOM	3449	OH2 TIP C		59.624	17.562	20.598	1.00 44.37
	3450	OH2 TIP C		40.644	39.227	19.932	1.00 37.57
ATOM	3451	OH2 TIP C		12.920	31.214	52.942	1.00 51.07
ATOM	3452	OH2 TIP C		37.639	0.847		1.00 49.44
		OH2 TIP C		34.243	38.790	-3.251	1.00 54.21
MOTA	3453					6.983	1.00 50.90
MOTA	3454	OH2 TIP C		24.216	47.874		
ATOM	3455	OH2 TIP C		15.324	34.797	6.670	
ATOM	3456	OH2 TIP C		18.474	15.525	21.402	1.00 34.12
MOTA	3457	OH2 TIP C		40.048	8.873	26.818	1.00 49.89
MOTA	3458	OH2 TIP C		32.472	13.331	20.523	1.00 29.86
MOTA	3459	OH2 TIP C		57.778	14.167	30.422	1.00 49.76
MOTA	3460	OH2 TIP C		46.651	35.476	13.375	1.00 56.48
ATOM	3461	OH2 TIP C		15.427	13.237	3.552	1.00 57.25
MOTA	3462	OH2 TIP C	342	40.349	38.972	3.722	1.00 65.27
ATOM	3463	OH2 TIP C		-8.685	28.945	15.205	1.00 59.60
ATOM	3464	OH2 TIP C		11.958	41.585	22.587	1.00 37.18
ATOM	3465	OH2 TIP C		9.054	20.498	28.914	1.00 42.95
ATOM	3466	OH2 TIP C		20.086	20.088	46.913	1.00 42.03
ATOM.	3467	OH2 TIP C		40.370	35.093	2.009	1.00 49.35
ATOM	3468	OH2 TIP C		41.948	4.327	12.147	1.00 50.59
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MOTA	3469	OH2	TIP	С	349	23.518	45.701	40.287	1.00	39.79
MOTA	3470	OH2	TIP	С	350	19.169	37.474	4.786	1.00	44.67
ATOM	3471	OH2	TIP	С	351	32.946	39.184	41.062	1.00	57.56
ATOM	3472	OH2	TIP	С	352	37.578	47.817	18.421	1.00	51.80
MOTA	3473	OH2	TIP	С	353	15.391	43.820	7.645	1.00	58.15
MOTA	3474	OH2	TIP	С	354	38.205	17.257	33.401	1.00	55.84
ATOM	3475	OH2	TIP	С	355	43.224	1.565	14.606	1.00	41.12
ATOM	3476	OH2	TIP	С	356	18.704	51.623	28.487	1.00	61.11
MOTA	3477	OH2	TIP	С	357	46.033	5.813	0.173	1.00	43.43
MOTA	3478	OH2	TIP	С	358	51.950	27.722	14.408	1.00	45.00
MOTA	3479	OH2	TIP	С	359	46.825	2.427	15.714	1.00	52.68
ATOM	3480	OH2	TIP	С	360	17.624	50.111	20.315	1.00	39.65
MOTA	3481	0	нон	С	361	27.534	15.877	26.687	1.00	20.00
MOTA	3482	0	нон	С	362	28.946	16.344	30.514	1.00	20.00
END										

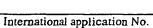
INTERNATIONAL SEARCH REPORT

International application No.

PCT/US01/29387

A. CLASSIFICATION OF SUBJECT MATTER IPC(7) G01N 33/483											
US CL	: 702/19		10 11 1100								
	International Patent Classification (IPC) or to both n	ational cia	assification and IPC								
B. FIELI	DS SEARCHED										
	Minimum documentation searched (classification system followed by classification symbols) U.S.: 702/17, 435, 424.										
Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched											
Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) Please See Continuation Sheet											
C. DOCI	UMENTS CONSIDERED TO BE RELEVANT										
Category *	Citation of document, with indication, where ap	propriate	, of the relevant passages	Relevant to claim No.							
Y											
Y ZHANG Z. et al. Sequence-specific recognition of the interanalization motif of the Alzheimer's amyloid precursor protein by the X11 PTB domain. The EMBO Journal. 1997, Vol 16. No. 20, pages 6141-6150, see entire document and especially page 6147.											
Y,P	MARCINKEVICIENE J. at al. Mechanism of Inhib Protein-cleaving Enzyme (BACE) by a Statine-base Chemistry. 29 June 2001, Vol 276, No. 26, pages 2	d Peptide	. The Journal of Biological	1							
Y	HYNES et al. X-ray Crystal Structure of the Protea Amyloid beta-Protein Precursor. Biochemistry 1990 especially page 10019.			1-2							
·-				,							
	·										
Further	r documents are listed in the continuation of Box C.		See patent family annex.								
* S	pecial categories of cited documents:	"T"	later document published after the int								
	t defining the general state of the art which is not considered to be		date and not in conflict with the appli principle or theory underlying the inv	ention							
	oplication or patent published on or after the international filing date	"X"	document of particular relevance; the considered novel or cannot be conside when the document is taken alone								
establish specified	•	"Y"	document of particular relevance; the considered to involve an inventive ste combined with one or more other suc	p when the document is h documents, such combination							
"O" documen	t referring to an oral disclosure, use, exhibition or other means		being obvious to a person skilled in the	ne art							
"P" document published prior to the international filing date but later than the "&" document member of the same patent family priority date claimed											
1	nctual completion of the international search r 2001 (18.12.2001)	Date of	mailing of the international sea	arch report 2002							
	vailing address of the ISA/US	Authori	zed officer	W > 0 / co-							
Cor Box	nmissioner of Patents and Trademarks PCT		Juya Dride	ALIZE OF LD							
Washington, D.C. 20231 Facsimile No. (703)305-3230 Telephone No. (703)-308-0196											

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INTERNATIONAL SEARCH REPORT PCT/US01/29387

C. (Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	BAILEY et al. X-ray-crystallographic studies of complexes of pepstatin A and a statine-containing human renin inhibitor with endothiapepsin. Biochem. J.1993, Vol 289, pages 363-371, especially pages 365-366.	1-2
Y	SCHEIDIG et al. Crystal structures of bovin chymotrypsin and trypsin complexed to the inhibitor domain of Alzheimer's amyloid beta-protein precursor (APPI) and basic pancreatic trypsin inhibitor (BPTI): Engineering of inhibitors wth altered specificities. The Protein Society. September 1997, Vol 6, pages 1806-1824, see entire document and especially page 1820.	1-2
Α	KOHNO et al. Thre-Dimentional Structure of the Amyloid beta Peptide (25-35) in Membrane-Mimicking Environment. Biochemistry. 1996, Vol 35, pages 16094-16104, see entire document.	1-2
Α	VASSAR et al. Beta-Secretase Cleavage of Azheimer's Amyloid Precursor Protein by the Transmembrane Aspartic Protease BACE. Science. 22 October 1999, Vol 286, pages 735-741, see entire document.	1-2
Α	HONG, L. et al. Structure of the Protease Domain of Memapsin 2(beta-Secretase) Complexed with Inhibitor. Science. 24 May 2000, Vol 290, No. 5489, pages 150-159, see entire document	1-2
A	SAUDER, M. et al. Modeling of substrate specifity of the Alzheimer's desease amyloid precursor protein beta-secretase. J. Mol. Biol. 2000, Vol 300, No. 2, pages 241-248, see entire document.	1-2
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INTERNATIONAL SEARCH REPORT

International application No.

PCT/US01/29387

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)				
This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:				
1.		Claim Nos.: because they relate to subject matter not required to be searched by this Authority, namely:		
2.		Claim Nos.: because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:		
3.	6.4(a).	Claim Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule		
Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)				
This International Searching Authority found multiple inventions in this international application, as follows: Please See Continuation Sheet				
1.		As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.		
2.		As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.		
3.		As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.: 1 and 2		
4.		No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:		
Rem	ark on l			
		No protest accompanied the payment of additional search fees.		

Form PCT/ISA/210 (continuation of first sheet(1)) (July 1998)



International application No.

PCT/US01/29387

BOX II. OBSERVATIONS WHERE UNITY OF INVENTION IS LACKING

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Invention I and II are directed to different chemical and physical types regarding the critical limitations therein. For Group I, the critical feature is a crystallization of complex whereas for Group II the critical feature is the obtaining or synthesizing the agent. This application contains the following inventions or groups of inventions which are not so linked as to form a single general inventive concept under PCT Rule 13.1. In order for all inventions to be searched, the appropriate additional examination fees must be paid.

Group I, claims 1-2, drawn to crystallized complex.

Group II, claims 24 and 27 drawn to method further comprising one of the steps: obtaining and synthesizing the agen. Claims 3-23, 25, 26, 28-30 are directed solely to information and are therefore excluded from search.

The International Searching Authority considers that the international application does not comply with the requirements of unity of invention (Rules 13.1, 13.2 and 13.3) for reasons indicated below:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Invention I and II are directed to different chemical and physical types regarding the critical limitations therein. For Group I, the critical feature is a crystallization of complex whereas for Group II the critical feature is the obtaining or synthesizing the agent.

Continuation of B. FIELDS SEARCHED Item 3:

WEST, STN, Non-patent-literature covering search terms: Cleaving Enzyme(BACE), crystallization, beta-Amyloid Precursor protein, 3-d structure of APP, Statine-based peptides.